# Package 'spaMM'

June 10, 2024

Type Package

Title Mixed-Effect Models, with or without Spatial Random Effects

**Encoding UTF-8** 

Version 4.5.0

Date 2024-06-09

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**Imports** methods, stats, graphics, Matrix, MASS, proxy, Rcpp (>= 0.12.10), nlme, nloptr, minqa, pbapply, crayon, gmp (>= 0.6.0), ROI, boot, geometry (>= 0.4.0), numDeriv, backports

**LinkingTo** Rcpp, RcppEigen (>= 0.3.3.5.0)

**Depends** R (>= 3.5.0)

**Suggests** maps, testthat, rcdd, foreach, future, future.apply, RANN, Infusion (>= 1.3.0), IsoriX (>= 0.8.1), blackbox (>= 1.1.25), RSpectra, ROI.plugin.glpk, lme4, rsae, multilevel, agridat

Enhances multcomp, RLRsim, lmerTest

**NeedsCompilation** yes

SystemRequirements GNU Scientific Library (GSL)

# **Description**

Inference based on models with or without spatially-correlated random effects, multivariate responses, or non-Gaussian random effects (e.g., Beta). Variation in residual variance (heteroscedasticity) can itself be represented by a mixed-effect model. Both classical geostatistical models (Rousset and Ferdy 2014 <doi:10.1111/ecog.00566>), and Markov random field models on irregular grids (as considered in the 'INLA' package, <https://www.r-inla.org>), can be fitted, with distinct computational procedures exploiting the sparse matrix representations for the latter case and other autoregressive models. Laplace approximations are used for likelihood or restricted likelihood. Penalized quasi-likelihood and other variants discussed in the h-likelihood literature (Lee and Nelder 2001 <doi:10.1093/biomet/88.4.987>) are also implemented.

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URL https://www.r-project.org,

https://gitlab.mbb.univ-montp2.fr/francois/spamm-ref

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Repository CRAN
<b>Date/Publication</b> 2024-06-09 22:20:02 UTC

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Simulated data set for testing sparse-precision code

Description

adjlg

This is used in tests/test-adjacency-long.R

# Usage

data("adjlg")

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#### **Format**

Includes an adjacency matrix adjlgMat. and a data frame adjlg with 5474 observations on the following 8 variables.

ID a factor with levels 1 to 1000 months a numeric vector
GENDER a character vector
AGE a numeric vector
X1 a numeric vector
X2 a numeric vector
month a numeric vector
BUY a numeric vector

#### Source

The simulation code shown below is derived from an example produced by Jeroen van den Ochtend. Following a change incorporated in spaMM version 3.8.0, that implied stricter checks of the input matrix, it appeared that the precision matrix generated by this example had inappropriate (repeated) dimnames. This example was then updated to reproduce past fitting results with a correctly formatted matrix. Note that changing the names of an adjacency matrix (as below) is generally unwise as it generally changes the statistical model because these names are matched whenever possible to levels of the grouping factor in the data.

The code was also modified to compensate for changes in R's default random number generator.

```
data(adjlg)
## See further usage in tests/test-adjacency-long.R
## Not run:
# as produced by:
 library(data.table) ## Included data produced using version 1.10.4.3
 library(igraph) ## Included data produced using version 1.2.1
 rsample <- function(N=100, ## size of implied adjacency matrix</pre>
                       month_max=10, seed) {
    if (is.integer(seed)) set.seed(seed)
    dt <- data.table(ID=factor(1:N))</pre>
    dt$months <- sample(1:month_max,N,replace=T) ## # of liens for each level of ID
    dt$GENDER <- sample(c("MALE", "FEMALE"), N, replace=TRUE)</pre>
    dt$AGE <- sample(18:99,N,replace=T)</pre>
    dt$X1 <- sample(1000:9900, N, replace=T)
    dt$X2 <- runif(N)</pre>
    dt <- dt[, c(.SD, month=data.table(seq(from=1, to=months, by = 1))), by = ID]
    dt[,BUY := 0]
    dt[month.V1==months,BUY := sample(c(0,1),1),by=ID]
    setnames(dt, "month.V1", "month")
```

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```
#### create adjacency matrix
    Network <- data.table(OUT=sample(dt$ID,N*month_max*4/10))</pre>
    Network$IN <- sample(dt$ID,N*month_max*4/10)</pre>
    Network <- Network[IN != OUT]</pre>
   Network <- unique(Network)</pre>
    g <- graph.data.frame(Network,directed=F)</pre>
    g <- add_vertices(g,sum(!unique(dt$ID) %in% V(g)),</pre>
             name=unique(dt[!dt$ID %in% V(g),list(ID)])) # => improper names
    Network <- as_adjacency_matrix(g,sparse = TRUE,type="both")</pre>
    colnames(Network) <- rownames(Network) <- seq(nrow(Network)) # post-v3.8.0 names</pre>
    return(list(data=dt,adjMatrix=Network))
 RNGkind("Mersenne-Twister", "Inversion", "Rounding" )
 set.seed(123)
 adjlg_sam <- rsample(N=1000, seed=NULL)</pre>
 RNGkind("Mersenne-Twister", "Inversion", "Rejection" )
 adjlg <- as.data.frame(adjlg_sam$data)</pre>
 adjlgMat <- adjlg_sam$adjMatrix</pre>
## End(Not run)
```

AIC

Extractors for information criteria such as AIC

# **Description**

get\_any\_IC computes model selection/information criteria such as AIC. See Details for more information about these criteria. The other extractors AIC and extractAIC are methods for HLfit objects of generic functions defined in other packages: AIC is equivalent to get\_any\_IC (for a single fitted-model object), and extractAIC returns the marginal AIC and the number of degrees of freedom for the fixed effects.

# Usage

#### **Arguments**

object, fit A object of class HLfit, as returned by the fitting functions in spaMM.

Scale, k Currently ignored, but are required in the definitions for consistency with the generic.

verbose Whether to print the model selection criteria or not.

Whether to include the plug-in estimate of conditional AIC in the result (its also\_cAIC

computation may be slow).

nsim Controls whether to include the bootstrap estimate of conditional AIC (see De-

tails) in the result. If positive, nsim gives the number of bootstrap replicates.

short.names NULL, or boolean; controls whether the return value uses short names (mAIC,

> etc., as shown by screen output if verbose is TRUE), or the descriptive names ("marginal AIC:", etc.) also shown in the screen output. Short names are more appropriate for programming but descriptive names may be needed for back-compatibility. The default (NULL) ensures back-compatibility by using

> descriptive names unless the bootstrap estimate of conditional AIC is reported.

For AIC.HLfit: may include more fitted-model objects, consistently with the generic. For this and the other functions: other arguments that may be needed by some method. For example, if nsim is positive, a seed argument may be passed to simulate, and the other "..." may be used to control the optional parallel execution of the bootstrap computations (by providing arguments to dopar).

#### **Details**

The AIC is a measure (by Kullback-Leibler directed distance, up to an additive constant) of quality of prediction of new data by a fitted model. Comparing information criteria may be viewed as a fast alternative to a comparison of the predictive accuracy of different models by cross-validation. Further procedures for model choice may also be useful (e.g. Williams, 1970; Lewis et al. 2010).

The **conditional AIC** (Vaida and Blanchard 2005) applies the AIC concept to new realizations of a mixed model, conditional on the realized values of the random effects. Lee et al. (2006) and Ha et al (2007) defined a corrected AIC [i.e., AIC(D\*) in their eq. 7] which is here interpreted as the conditional AIC.

Such Kullback-Leibler relative distances cannot generally be evaluated exactly and various estimates have been discussed. get\_any\_IC computes, optionally prints, and returns invisibly one or more of the following quantities:

- \* Akaike's classical AIC (marginal AIC, mAIC, i.e., minus twice the marginal log-likelihood plus twice the number of fitted parameters);
- \* a plug-in estimate (cAIC) and/or a bootstrap estimate (b\_cAIC) of the conditional AIC;
- \* a focussed AIC for dispersion parameters (dispersion AIC, dAIC).

For the **conditional AIC**, Vaida and Blanchard's plug-in estimator involves the conditional likelihood, and degrees of freedom for (i) estimated residual error parameters and (ii) the overall linear predictor characterized by the Effective degrees of freedom already discussed by previous authors including Lee and Nelder (1996), which gave a plug-in estimator  $(p_D)$  for it in HGLMs. By default, the plug-in estimate of both the conditional AIC and of  $n-p_D$  (GoFdf, where n is the length of the response vector) are returned by get\_any\_IC. But these are biased estimates of conditional AIC and effective df, and an alternative procedure is available for GLM response families if a non-default positive nsim value is used. In that case, the conditional AIC is estimated by a bootstrap version of Saefken et al. (2014)'s equation 2.5; this involves refitting the model to each bootstrap samples, so it may take time, and a full cross-validation procedure might as well be considered for model selection.

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The dispersion AIC has been defined from restricted likelihood by Ha et al (2007; eq.10). The present implementation will use restricted likelihood only if made available by an REML fit, otherwise marginal likelihood is used.

#### Value

get\_any\_IC, a numeric vector whose possible elements are described in the Details, and whose names are controlled by the short.names argument. Note that the bootstrap computation actually makes sense and works also for fixed-effect models (although it is not clear how useful it is in that case). The return value will still refer to its results as conditional AIC.

For AIC, If just one fit object is provided, the same return value as for get\_any\_IC. If multiple objects are provided, a data.frame built from such vectors, with rows corresponding to the objects.

For extractAIC, a numeric vector of length 2, with first and second elements giving

 $\star$  edf the degree of freedom of the fixed-effect terms of the model for the fitted model fit.

\* AIC the (marginal) Akaike Information Criterion for fit.

Likelihood is broadly defined up to a constant, which opens the way for inconsistency between different likelihood and AIC computations. In **spaMM**, likelihood is nothing else than the probability or probability density of the data as function of model parameters. No constant is ever added, in contrast to stats::extractAIC output, so there are discrepancies with the latter function (see Examples).

## References

Ha, I. D., Lee, Y. and MacKenzie, G. (2007) Model selection for multi-component frailty models. Statistics in Medicine 26: 4790-4807.

Lee Y. and Nelder. J. A. 1996. Hierarchical generalized linear models (with discussion). J. R. Statist. Soc. B, 58: 619-678.

Lewis, F., Butler, A. and Gilbert, L. (2011), A unified approach to model selection using the likelihood ratio test. Methods in Ecology and Evolution, 2: 155-162. doi:10.1111/j.2041210X.2010.00063.x

Saefken B., Kneib T., van Waveren C.-S., Greven S. (2014) A unifying approach to the estimation of the conditional Akaike information in generalized linear mixed models. Electron. J. Statist. 8, 201-225.

Vaida, F., and Blanchard, S. (2005) Conditional Akaike information for mixed-effects models. Biometrika 92, 351-370.

Williams D.A. (1970) Discrimination between regression models to determine the pattern of enzyme synthesis in synchronous cell cultures. Biometrics 26: 23-32.

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```
as a result of the previous computation, and is now returned even by:
get_any_IC(m1, also_cAIC=FALSE)
if (spaMM.getOption("example_maxtime")>4) {
get_any_IC(m1, nsim=100L, seed=123) # provides bootstrap estimate of cAIC.
# (parallelisation options could be used, e.g. nb_cores=detectCores(logical=FALSE)-1L)
}
extractAIC(m1)
## Not run:
# Checking (in)consistency with glm example from help("stats::extractAIC"):
utils::example(glm) # => provides 'glm.D93' fit object
logLik(glm.D93) # logL= -23.38066 (df=5)
dataf <- data.frame(counts=counts,outcome=outcome, treatment=treatment)</pre>
extractAIC(fitme(counts ~ outcome + treatment, family = poisson(), data=dataf))
\# => 56.76132 = -2 logL + 2* df
extractAIC(glm.D93) # 56.76132 too
#
# But for LM:
lm.D93 <- lm(counts ~ outcome + treatment, data=dataf)</pre>
logLik(lm.D93) # logL=-22.78576 (df=6)
extractAIC(fitme(counts \sim outcome + treatment, data=dataf)) # 57.5715 = -2 logL + 2* df
extractAIC(1m.D93) # 30.03062
### Inconsistency also apparent in drop1 output for :
# Toy data from McCullagh & Nelder (1989, pp. 300-2), as in 'glm' doc:
clotting <- data.frame(</pre>
   u = c(5,10,15,20,30,40,60,80,100),
   lot1 = c(118, 58, 42, 35, 27, 25, 21, 19, 18),
   lot2 = c(69, 35, 26, 21, 18, 16, 13, 12, 12))
drop1( fitme(lot1 ~ log(u), data = clotting), test = "F") # agains reports marginal AIC
# => this may differ strongly from those returned by drop1( < glm() fit > ),
# but the latter are not even consistent with those from drop1( < lm() fit > )
# for linear models. Compare
drop1(lm(lot1 \sim log(u), data = clotting), test = "F") # consistent with drop1.HLfit()
drop1( glm(lot1 ~ log(u), data = clotting), test = "F") # inconsistent
## Discrepancies in drop1 output with Gamma() family:
gglm <- glm(lot1 ~ 1, data = clotting, family=Gamma())</pre>
logLik(gglm) # -40.34633 (df=2)
spgglm <- fitme(lot1 ~ 1, data = clotting, family=Gamma())</pre>
logLik(spgglm)
                                     # -40.33777 (slight difference:
# see help("method") for difference in estimation method between glm() and fitme()).
# Yet this does not explain the following:
drop1( fitme(lot1 ~ log(u), data = clotting, family=Gamma()), test = "F")
# => second AIC is 84.676 as expected from above logLik(spgglm).
drop1( glm(lot1 \sim log(u), data = clotting, family=Gamma()), test = "F")
# => second AIC is 1465.27, quite different from -2*logLik(gglm) + 2*df
```

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## End(Not run)

algebra

Control of matrix-algebraic methods

# **Description**

Autocorrelated gaussian random effects can be specified in terms of their covariance matrix, or in terms of the precision matrix (i.e. inverse covariance matrix). In a pre-processing step, spaMM may assess whether such precision matrices are sparse but the correlation matrix is dense, and if so, it may use "sparse-precision" algorithms efficient for this case. If the precision matrix does not appear sufficiently sparser than the correlation matrix, correlation matrices are used, and they can themselves be sparse or dense, with distinct algebraic methods used in each case.

For example, when the model includes a corrMatrix term specified by a covariance matrix, the precision matrix may be computed to assess its sparseness. The Example below illustrates a case where detecting sparsity of the precision matrix allows a faster fit. However, such a comparison of correlation and precision matrices takes time and is not performed for all types of random-effect structures. Instead, some fast heuristics may be used (see Details). The default selection of methods may not always be optimal, and may be overcome by using the control.HLfit argument of the fitting function (or by spaMM.options(), see Details). In particular one can use either control.HLfit=list(sparse\_precision= <TRUE|FALSE>) or control.HLfit=list(algebra= <"spprec"|"spcorr"|"decorr">) with the obvious expected effects.

Such control may be useful when you already know that the precision matrix is sparse (as spaMM may even kindly remind you of, see Example below). In that case, it is also efficient to specify the precision matrix directly (see Example in Gryphon), as spaMM then assumes that sparse-precision methods are better without checking the correlation matrix.

Such control may also be useful when the correlation matrix is nearly singular so that computation of its inverse fails. This may occur if the model is poorly specified, but also occurs sometimes for valid correlation models because inversion of large matrices though Cholesky methods is not numerically accurate enough. In the latter case, you may be directed to this documentation by an error message, and specifying sparse\_precision= FALSE may be useful.

# **Details**

Currently the sparse-precision methods are selected by default in two cases (with possible exceptions indicated by specific messages): (1) for models including IMRF random effects; and (2) when the corrMatrix (or covStruct) syntax is used to provide a fixed precision matrix. Further, for models including autoregressive terms other than IMRF (i.e., adjacency, AR1), sparse-precision methods may or may not be selected on a simple heuristic based on the likely structure of the correlation matrix.

Algebraic methods can be controlled globally over all further fits by using spaMM.options(sparse\_precision= <TRUE|FALSE>) and, among the correlation-based methods,

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```
spaMM.options(QRmethod=<"sparse"|"dense">)
to select "spcorr" vs. "decorr" methods. Fit-specific controls (by control.HLfit) override these
global ones.
```

#### See Also

pedigree

# **Examples**

arabidopsis

Arabidopsis genetic and climatic data

# **Description**

For 948 "accessions" from European Arabidopsis thaliana populations, this data set merges the genotypic information at four single nucleotide polymorphisms (SNP) putatively involved in adaptation to climate (Fournier-Level et al, 2011, Table 1), with 13 climatic variables from Hancock et al. (2011).

#### **Usage**

```
data("arabidopsis")
```

# **Format**

The data frame includes 948 observations on the following variables:

pos1046738, pos5510910, pos6235221, pos8132698 Genotypes at four SNP loci

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LAT latitude

LONG longitude

seasonal, tempWarmest, tempColdest, preciWettest, preciDriest, preciCV, PAR\_SPRING,

growingL, conseqCold, conseqFrFree, RelHumidSp, dayLSp, aridity Thirteen climatic variables. See Hancock et al. (2011) for details about these variables.

#### **Details**

The response is binary so method="PQL/L" seems warranted (see Rousset and Ferdy, 2014).

#### Source

The data were retrieved from http://bergelson.uchicago.edu/regmap-data/climate-genome-scan on 22 February 2013 (they may no longer be available from there).

#### References

Fournier-Level A, Korte A., Cooper M. D., Nordborg M., Schmitt J., Wilczek AM (2011). A map of local adaptation in Arabidopsis thaliana. Science 334: 86-89.

Hancock, A. M., Brachi, B., Faure, N., Horton, M. W., Jarymowycz, L. B., Sperone, F. G., Toomajian, C., Roux, F., and Bergelson, J. 2011. Adaptation to climate across the Arabidopsis thaliana genome, Science 334: 83-86.

Rousset F., Ferdy, J.-B. (2014) Testing environmental and genetic effects in the presence of spatial autocorrelation. Ecography, 37: 781-790. doi:10.1111/ecog.00566

ARp 13

ARp	Random effect with $AR(p)$ (autoregressive of order $p$ ) or $ARMA(p,q)$
	structure.

# Description

These times-series correlation models can be declared as correlation models for random effect. The AR(p) model is here parametrized by the **partial** correlation coefficients of the levels of the random effect,  $\{U_t\}$ ,  $corr(U_s,U_t|U_s+1),...,U_t-1)$ , with valid values in the hypercube ]-1,,1[^p (Barndorff-Nielsen and Schou, 1973). In the autoregressive-moving average ARMA(p,q) model, the AR part is parametrized in the same way. AR parameters are named "p1", "p2"..., and MA parameters are named "q1", "q2"....

Implementation of the AR(p) model uses the sparsity of the inverse covariance matrix. In the ARMA(p,q) model, neither the covariance nor its inverse are sparse, so fits are expected to be more time- and memory-consuming.

# Usage

```
# corrFamily constructors:
ARp(p=1L, fixed=NULL, corr=TRUE, tpar=1/(1+seq(p)))
ARMA(p=1L, q=1L, fixed=NULL, tpar=c(1/(1+seq_len(p)),1/(1+seq_len(q))))
```

# **Arguments**

p	Integer: order of the autoregressive process.
q	Integer: order of the moving-average process.
tpar	Numeric vector: template values of the <b>partial coefficient coefficients</b> of the autoregressive process, and the traditional coefficients of the moving-average processe, in this order. The tpar vector must always have full length, even when some parameters are fixed.
fixed	NULL or numeric vector, to fix the parameters of this model.
corr	For development purposes, better ignored in normal use.

## Value

The ARp and ARMA functions return a corrFamily descriptor, hence a list including element Cf, a function returning, for given ARMA or AR parameters, the correlation matrix for ARMA, or its **inverse** for ARp.

The fitted correlation matrix can be extracted from a fit object, as for any autocorrelated random effect, by Corr(<fit object>)[[<random-effect index>]].

# References

Barndorff-Nielsen 0. and Schou G., 1973 On the parametrization of autoregressive models by partial autocorrelations. J. Multivariate Analysis 3: 408-419. doi:10.1016/0047259X(73)900304

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### **Examples**

```
if (spaMM.getOption("example_maxtime")>2) {
ts <- data.frame(lh=lh,time=seq(48)) ## using 'lh' data from 'stats' package
## Default 'tpar' => AR1 model
(ARpfit <- fitme(lh ~ 1 + ARp(1|time), data=ts, method="REML"))
## which is equivalent to
(AR1fit <- fitme(lh ~ 1 +AR1(1|time), data=ts, method="REML"))
## AR(3) model
(AR3fit <- fitme(lh ~ 1 + ARp(1|time, p=3), data=ts, method="REML"))
## Same but with fixed 2-lag partial autocorrelation
(AR3fix \leftarrow fitme(1h \sim 1 + ARp(1|time, p=3, fixed=c(p2=0)), data=ts, method="REML"))
# The fit should be statistically equivalent to
(AR3_fix <- fitme(lh ~ 1 + ARp(1|time, p=3), data=ts, method="REML",
                 fixed=list(corrPars=list("1"=c(p2=0)))))
# with subtle differences in the structure of the fit objects:
get_ranPars(AR3fix)$corrPars
                                 # p2 was not a parameter of the model
get_ranPars(AR3_fix)$corrPars
                                 # p2 was a fixed parameter of the model
# get_fittefPars() expectedly ignores 'p2' whichever way it was fixed.
## Same as 'AR3fix' but with an additional MA(1) component
(ARMAfit \leftarrow fitme(lh \sim 1 + ARMA(1|time, p=3, q=1, fixed=c(p2=0)),
                  data=ts, method="REML"))
}
```

as\_LMLT

Conversion to input for procedures from lmerTest package

# **Description**

The lmerTest::contest function, drop1 and anova methods implement a number of tests for linear mixed models, e.g. using effective degrees of freeedom based on (a generalization of) Satterthwaite's method. These tests can be performed using **spaMM** fits through the conversion of the

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fit object, by the as\_LMLT function, to an ad-hoc format acceptable as input to **lmerTest**'s internal procedures. The separately documented drop1.HLfit and (optionally) anova.HLfit methods, when called on a single LMM fit object, perform the conversion by as\_LMLT and call drop1 or anova methods defined by **lmerTest**.

Only the tests using **lmerTest**'s default method ddf="Satterthwaite" are formally supported, as the converted object do not have the required format for the other methods. Only LMMs are handled by **lmerTest**, and residual-dispersion models are not yet handled by the conversion. However, the conversion extends **lmerTest**'s functionality by handling all random-effect parameters handled by numInfo, therefore including (e.g.) spatial-correlation parameters not handled by **lme4**.

# Usage

```
as_LMLT(fitobject, nuisance=NULL, verbose=TRUE, transf=TRUE, check_deriv=NULL, ...)
```

#### **Arguments**

fitobject	Object of class HLfit resulting from the fit of a linear mixed model (LMM).
nuisance	A list of fitted values of parameters that affect the distribution of the test of fixed effects, in the format of the fixed argument of the fitme function. If NULL (default), then the list is constructed from the fitted values of the random-effect parameters and of phi (residual dispersion parameter). The nuisance argument is better ingored unless the extractor he construct the default value fails in some way.
verbose	boolean: controls printing of the message that shows the unlisted value of the nuisance list.
transf	boolean: whether to evaluate numerical derivatives on a transformed parameter scale, or not (may affect numerical precision).
check_deriv	See same-named argument of numInfo
	Other arguments that may be needed by some method (currently ignored).

# Value

The value is returned invisibly. It is an S4 object of class "LMLT" with slots matching those required in objects of S4 class "lmerModLmerTest" when used by package **lmerTest** with ddf="Satterthwaite" (many additional slots of a formal "lmerModLmerTest" object are missing). The additional nuisance slot contains the nuisance list.

# References

Alexandra Kuznetsova, Per B. Brockhoff and Rune H. B. Christensen (2017) ImerTest Package: Tests in Linear Mixed Effects Models. Journal of Statistical Software, 82(13), 1–26. doi:10.18637/jss.v082.i13

```
## Reproducing an example from the doc of lmerTest::contest.lmerModLmerTest,
# using a spaMM fit as input.
## Not run:
data("sleepstudy", package="lme4")
```

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autoregressive

Fitting autoregressive models

#### **Description**

Diverse autoregressive (AR) models are implemented in spaMM. This documentation describe the adjacency model (a conditional AR, i.e., CAR), and the AR1 model for time series. Other documentation deals with more or less distantly related models: ARp for more general AR(p) and ARMA(p,q) models for time series, and IMRF and MaternIMRFa for mesh-based approximations of geostatistical models.

An AR1 random effect is specified as AR1(1|<grouping factor>). It describes correlations between realizations of the random effect for (typically) successive time-steps by a correlation  $\phi$ , denoted ARphi in function calls. Nested AR1 effects can be specified by a nested grouping factor, as in AR1(1|<time index> %in% <nesting factor>).

A CAR random effect is specified as adjacency(1|<grouping factor>). The correlations among levels of the random effect form a matrix  $(\mathbf{I}-\rho \text{ adjMatrix})^{-1}$ , in terms of an adjMatrix matrix which must be provided, and of the scalar  $\rho$ , denoted rho in function calls. The rows and columns of adjMatrix must have names matching those of levels of the random effect **or else** are assumed to match a sequence, from 1 to the number of columns, of values of the geographic location index specifying the spatial random effect. For example, if the model formula is

 $y \sim adjacency(1|geo.loc)$  and data>geo.loc is 2,4,3,1,... the first row/column of the matrix refers to geo.loc=1, i.e. to the fourth row of the data.

#### **Details**

Efficient algorithms for CAR models have been widely discussed in particular in the econometric literature (e.g., LeSage and Pace 2009), but these models are not necessarily recommended for irregular lattices (see Wall, 2004 and Martellosio, 2012 for some insights on the implications of autoregressive models).

In **CAR** models, the covariance matrix of random effects  $\mathbf{u}$  can be described as  $\lambda(\mathbf{I}-\rho \mathbf{W})^{-1}$  where  $\mathbf{W}$  is the (symmetric) adjacency matrix. HLCor uses the spectral decomposition of the adjacency

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matrix, written as **W=VDV**' where **D** is a diagonal matrix of eigenvalues  $d_i$ . The covariance of  $\mathbf{V}$ ' $\mathbf{u}$  is  $\lambda(\mathbf{I}-\rho\,\mathbf{D})^{-1}$ , which is a diagonal matrix with elements  $\lambda_i=\lambda/(1-\rho d_i)$ . Hence  $1/\lambda_i$  is in the linear predictor form  $\alpha+\beta d_i$  This can be used to fit  $\lambda$  and  $\rho$  efficiently. A call to corrHLfit with the additional argument init.HLfit=list(rho=0) should be equivalent in speed and result to the HLCor call.

This is fast for small datasets (as in the example below) but more generic maximization algorithms may be preferable for large ones. It is suggested to use fitme generally unless one has a large number of small data sets to analyze. A call to fitme or corrHLfit without that initial value does not use the spectral decomposition. It performs numerical maximization of the likelihood (or restricted likelihood) as function of the correlation parameter  $\rho$ . The choice of fitting function may slightly impact the results. The ML fits by corrHLfit and HLCor should be practically equivalent. The REML fits should slightly differ from each other, due to the fact that the REML approximation for GLMMs does not maximize a single likelihood function.

If HLCor is used, the results are reported as the coefficients  $\alpha$  ((Intercept)) and  $\beta$  (adjd) of the predictor for  $1/\lambda_i$ , in addition to the resulting values of  $\rho$  and of the common  $\lambda$  factor.

Different fits may also differ in using or not algorithms that exploit the sparsity of the precision matrix of the autoregressive random effect. By default, spaMM tends to select sparse-precision algorithms for large datasets and large (i.e. many-level) random effects (details are complex). However, for **AR1** models, the dimension of the implied precision matrix is determined by the extreme values of grouping factor (typically interpreted as a time index), as all intermediate values must be considered. Then, the correlation-based algorithms may be more efficient if only a few levels are present in the data, as only a small correlation matrix is required in that case.

#### References

LeSage, J., Pace, R.K. (2009) Introduction to Spatial Econometrics. Chapman & Hall/CRC.

Martellosio, F. (2012) The correlation structure of spatial autoregressions, Econometric Theory 28, 1373-1391.

Wall M.M. (2004) A close look at the spatial structure implied by the CAR and SAR models: Journal of Statistical Planning and Inference 121: 311-324.

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```
adjMatrix=Nmatrix, family=poisson(), data=scotlip, method="ML")
```

betabin

Beta-binomial family object

# **Description**

Returns a family object for beta-binomial models. The model described by such a family is characterized by a linear predictor, a link function, and the beta-binomial distribution for residual variation.

The precision parameter prec of this family is a positive value such that the variance of the betadistributed latent variable given its mean  $\mu$  is  $\mu(1-\mu)/(1+\text{prec})$ . prec is thus the same precision parameter as for the beta response family (see beta\_resp. The variance of the beta-binomial sample of size n is response is  $\mu(1-\mu)n(n+\text{prec})/(1+\text{prec})$ .

A fixed-effect residual-dispersion model can be fitted, using the resid.model argument, which is used to specify the form of the logarithm of the precision parameter (see Examples). Thus the variance of the latent beta-distributed variable becomes  $\mu(1-\mu)/(1+\exp(<\operatorname{specified linear expression}))$ .

#### **Usage**

```
betabin(prec = stop("betabin's 'prec' must be specified"), link = "logit")
```

# **Arguments**

link

prec Scalar (or left unspecified): precision parameter of the beta distribution.

logit, probit, cloglog or cauchit link, specified by any of the available ways for

GLM links (name, character string, one-element character vector, or object of

class link-glm as returned by make.link).

## **Details**

Prior weights are meaningful for this family and handled as a factor of the precision parameter of the latent beta-distributed variable: the variance of the latent variable become  $\mu(1-\mu)/(1+\text{prec}*<\text{prior weights}>)$ . However, this feature is experimental and may be removed in the future. The fitting function's resid.model argument may be preferred to obtain the same effect, by specifying an offset(log(<prior weights>)) in its formula (given the log link used in that model). As usual in **spaMM**, the offset(.) argument should be a vector and any variable necessary for evaluating it should be in the data.

## Value

A list, formally of class c("LLF", "family"). See LL-family for details about the structure and usage of such objects.

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### **Examples**

```
if (requireNamespace("agridat", quietly = TRUE)) {
   data("crowder.seeds", package = "agridat")
   fitme(cbind(germ,n-germ) ~ gen+extract+(1|plate), data=crowder.seeds, family=betabin())
} else {
   data(clinics)
   fitme(cbind(npos,nneg)~1+(1|clinic), family=betabin(), data=clinics)
}
```

beta\_resp

Beta-response family object

# Description

Returns a family object for beta-response models. The model described by such a family is characterized by a linear predictor, a link function, and the beta density for the residual variation.

The precision parameter prec of this family is a positive value such that the variance of the response given its mean  $\mu$  is  $\mu(1-\mu)/(1+\text{prec})$ . prec is thus the precision parameter  $\phi$  of Ferrari & Cribari-Neto (2004) and of the **betareg** package (Cribari-Neto & Zeileis 2010).

A fixed-effect residual-dispersion model can be fitted, using the resid.model argument, which is used to specify the form of the logarithm of the precision parameter (see Examples). Thus the variance of the response become  $\mu(1-\mu)/(1+\exp(<\operatorname{specified linear expression}>))$ .

# Usage

```
beta_resp(prec = stop("beta_resp's 'prec' must be specified"), link = "logit")
```

## Arguments

prec Scalar (or left unspecified): precision parameter of the beta distribution.

link logit, probit, cloglog or cauchit link, specified by any of the available ways for

GLM links (name, character string, one-element character vector, or object of

class link-glm as returned by make.link).

#### **Details**

Prior weights are meaningful for this family and handled as a factor of the precision parameter (as for GLM families) hence here not as a divisor of the variance (in contrast to GLM families): the variance of the response become  $\mu(1-\mu)/(1+\text{prec}*<\text{prior weights}>)$ . However, this feature is experimental and may be removed in the future. The fitting function's resid.model argument may be preferred to obtain the same effect, by specifying an offset(log(<prior weights>)) in its formula (given the log link used in that model). As usual in **spaMM**, the offset(.) argument should be a vector and any variable necessary for evaluating it should be in the data.

#### Value

A list, formally of class c("LLF", "family"). See LL-family for details about the structure and usage of such objects.

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#### References

Cribari-Neto, F., & Zeileis, A. (2010). Beta Regression in R. Journal of Statistical Software, 34(2), 1-24. doi:10.18637/jss.v034.i02

Ferrari SLP, Cribari-Neto F (2004). "Beta Regression for Modelling Rates and Proportions." Journal of Applied Statistics, 31(7), 799-815.

#### See Also

Further examples in LL-family.

# **Examples**

```
set.seed(123)
beta_dat <- data.frame(y=runif(100),grp=sample(2,100,replace = TRUE), x_het=runif(100))
fitme(y ~1+(1|grp), family=beta_resp(), data= beta_dat)
## same logL, halved 'prec' when prior weights=2 are used:
# fitme(y ~1+(1|grp), family=beta_resp(), data= beta_dat, prior.weights=rep(2,100))
## With model for residual dispersion:
# fitme(y ~1+(1|grp), family=beta_resp(), data= beta_dat, resid.model= ~ x_het)</pre>
```

blackcap

Genetic polymorphism in relation to migration in the blackcap

# Description

This data set is extracted from a study of genetic polymorphisms potentially associated to migration behaviour in the blackcap (Sylvia atricapilla). Across different populations in Europe and Africa, the average migration behaviour was found to correlate with average allele size (dependent on the number of repeats of a small DNA motif) at the locus ADCYAP1, encoding a neuropeptide. This data set is quite small and ill-suited for separating random-effect variance from residual variance. The likelihood surface for the Matérn model actually has local maxima.

# Usage

```
data("blackcap")
```

## **Format**

The data frame includes 14 observations on the following variables:

latitude latitude, indeed.

longitude longitude, indeed.

**migStatus** migration status as determined by Mueller et al, from 0 (resident populations) to 2.5 (long-distance migratory populations)

means Mean allele sizes in each population

pos Numerical index for the populations

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#### **Details**

Migration status was coded as: pure resident populations as '0', resident populations with some migratory restlessness as '0.5', partial migratory populations as '1', completely migratory populations migrating short-distances as '1.5', intermediate-distance migratory populations as '2' and distinct long-distance migratory populations as '2.5'.

#### Source

Data from Mueller et al. (2011), including supplementary material now available from doi:10.1098/rspb.2010.2567.

#### References

Mueller, J. C., Pulido, F., and Kempenaers, B. 2011. Identification of a gene associated with avian migratory behaviour, Proc. Roy. Soc. (Lond.) B 278, 2848-2856.

# **Examples**

```
## see 'fitme', 'corrHLfit' and 'fixedLRT' for examples involving these data
```

CauchyCorr

Cauchy correlation function and Cauchy formula term

# **Description**

The Cauchy family of correlation functions is useful to describe spatial processes with power-law decrease of correlation at long distance. It is valid for Euclidean distances in spaces of any dimension, and for great-circle distances on spheres of any dimension. It has a scale parameter (rho, as in the Matérn correlation function), a shape (or "smoothness", Gneiting 2013) parameter, and a long-memory dependence (or, more abstractly, "shape"; Gneiting 2013) parameter (Gneiting and Schlater 2004). The present implementation also accepts a Nugget parameter. The family can be invoked in two ways. First, the CauchyCorr function evaluates correlations, using distances as input. Second, a term of the form Cauchy(1|<...>) in a formula specifies a random effect with Cauchy correlation function, using coordinates found in a data frame as input. In the latter case, the correlations between realizations of the random effect for any two observations in the data will be the value of the Cauchy function at the scaled distance between coordinates specified in <...>, using "+" as separator (e.g., Cauchy(1|longitude+latitude)). A syntax of the form Cauchy(1|longitude+latitude %in% grp) can be used to specify a Cauchy random effect with independent realizations for each level of the grouping variable grp.

# Usage

```
## Default S3 method:
CauchyCorr(d, rho=1, shape, longdep, Nugget=NULL)
# Cauchy(1|...)
```

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#### **Arguments**

d Euclidean or great-circle distance

rho The scaling factor for distance, a real >0.

shape The shape (smoothness) parameter, a real 0<.<=2 for Euclidean distances and

0<.<=1 for great-circle distances. Smoothness increases, and fractal dimension decreases, with increasing shape (the fractal dimension of realizations in spaces

of dimension d being d+1-shape/2).

longdep The long-memory dependence parameter, a real >0. It gives the exponent of the

asymptotic decrease of correlation with distance: the smaller longdep is, the

longer the dependence.

Nugget (Following the jargon of Kriging) a parameter describing a discontinuous de-

crease in correlation at zero distance. Correlation will always be 1 at d=0, and

from which it immediately drops to (1-Nugget). Defaults to zero.

... Names of coordinates, using "+" as separator (e.g., Matern(1|longitude+latitude).

The coordinates are numeric values found in the data data frame provided to the fitting function. No additional declaration of groups, factors, or other specific

formatting is required.

#### **Details**

The correlation at distance d > 0 is

$$(1-{\rm Nugget})(1+(\rho d)^{\rm shape})^{(}-{\rm longdep/shape})$$

## Value

Scalar/vector/matrix depending on input.

### References

Gneiting, T. and Schlater M. (2004) Stochastic models that separate fractal dimension and the Hurst effect. SIAM Rev. 46: 269–282.

Gneiting T. (2013) Strictly and non-strictly positive definite functions on spheres. Bernoulli 19: 1327-1349.

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```
# See ?MaternCorr for examples of syntaxes for group-specific random effects,
# also handled by Cauchy().
```

clinics

Toy dataset for binomial response

# **Description**

A small data set used by Booth & Hobert (1998).

# Usage

```
data("clinics")
```

# **Format**

A data frame with 16 observations on the following 4 variables.

```
npos a numeric vector
nneg a numeric vector
treatment a numeric vector
clinic a numeric vector
```

#### References

Booth, J.G., Hobert, J.P. (1998) Standard errors of prediction in generalized linear mixed models. J. Am. Stat. Assoc. 93: 262-272.

```
data(clinics)
## Not run:
# The dataset was built as follows
npos <- c(11,16,14,2,6,1,1,4,10,22,7,1,0,0,1,6)
ntot <- c(36,20,19,16,17,11,5,6,37,32,19,17,12,10,9,7)
treatment <- c(rep(1,8),rep(0,8))
clinic <-c(seq(8),seq(8))
clinics <- data.frame(npos=npos,nneg=ntot-npos,treatment=treatment,clinic=clinic)
## End(Not run)</pre>
```

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COMPoisson

Conway-Maxwell-Poisson (COM-Poisson) GLM family

# Description

The COM-Poisson family is a generalization of the Poisson family which can describe over-dispersed as well as under-dispersed count data. It is indexed by a parameter nu that quantifies such dispersion. For nu>1, the distribution is under-dispersed relative to the Poisson distribution with same mean. It includes the Poisson, geometric and Bernoulli as special (or limit) cases (see Details). The COM-Poisson family is here implemented as a family object, so that it can be fitted by glm, and further used to model conditional responses in mixed models fitted by this package's functions (see Examples). nu is distinct from the dispersion parameter  $\nu=1/\phi$  considered elsewhere in this package and in the GLM literature, as  $\nu$  affects in a more specific way the log-likelihood.

Several links are now allowed for this family, corresponding to different versions of the COMPoisson described in the literature (e.g., Sellers & Shmueli 2010; Huang 2017).

# Usage

## Arguments

link GLM link function. The default is the canonical link "loglambda" (see Details),

but other links are allowed (currently log, sqrt or identity links as commonly

handled for the Poisson family).

nu Under-dispersion parameter. The fitme and corrHLfit functions called with

family=COMPoisson() (no given nu value) will estimate this parameter. In other usage of this family, nu must be specified. COMPoisson(nu=1) is the Pois-

son family.

#### **Details**

The ith term of the distribution can be written  $q_i/Z$  where  $q_i=\lambda^i/(i!)^\nu$  and  $Z=\sum_{(i=0)}^\infty q_i$ , for  $\lambda=\lambda(\mu)$  implied by its inverse relationship, the expectation formula  $\mu=\mu(\lambda)=\sum_{(i=0)}^\infty iq_i(\lambda)/Z$ . The case nu=0 is the geometric distribution with parameter  $\lambda$ ; nu=1 is the Poisson distribution with mean  $\lambda$ ; and the limit as nu ->  $\infty$  is the Bernoulli distribution with expectation  $\lambda/(1+\lambda)$ .

From this definition, this is an exponential family model with canonical parameters  $log(\lambda)$  and  $\nu$ . When the linear predictor  $\eta$  specifies  $log(\lambda(\mu))$ , the canonical link is used (e.g., Sellers & Shmueli 2010). It is here nicknamed "loglambda" and does not have a known expression in terms of elementary functions. To obtain  $\mu$  as the link inverse of the linear predictor  $\eta$ , one then first computes  $\lambda = e^{\eta}$  and then  $\mu(\lambda)$  by the expectation formula. For other links (Huang 2017), one directly computes  $\mu$  by the link inverse (e.g.,  $\mu = e^{\eta}$  for link "log"), and then one may solve for  $\lambda = \lambda(\mu)$  to obtain other features of the distribution.

The relationships between  $\lambda$  and  $\mu$  or other moments of the distribution involve infinite summations. These sums can be easily approximated by a finite number of terms for large nu but not when nu

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approaches zero. For this reason, the code may fail to fit distributions with nu approaching 0 (strong residual over-dispersion). The case nu=0 (the geometric distribution) is fitted by an ad hoc algorithm devoid of such problems. Otherwise, spaMM truncates the sum, and uses numerical integrals to approximate missing terms (which slows down the fitting operation). In addition, it applies an ad hoc continuity correction to ensure continuity of the result in nu=1 (Poisson case). These corrections affect numerical results for the case of residual overdispersion but are negligible for the case of residual underdispersion. Alternatively, spaMM uses Gaunt et al.'s (2017) approximations when the condition defined by spaMM. getOption("CMP\_asympto\_cond") is satisfied. All approximations reduces the accuracy of computations, in a way that can impede the extended Levenberg-Marquardt algorithm sometimes needed by spaMM.

The name COMP\_nu should be used to set initial values or bounds on nu in control arguments of the fitting functions (e.g., fitme(.,init=list(COMP\_nu=1))). Fixed values should be set by the family argument (COMPoisson(nu=.)).

#### Value

A family object.

#### References

Gaunt, Robert E. and Iyengar, Satish and Olde Daalhuis, Adri B. and Simsek, Burcin. (2017) An asymptotic expansion for the normalizing constant of the Conway–Maxwell–Poisson distribution. Ann Inst Stat Math doi:10.1007/s1046301706296.

Huang, Alan (2017) Mean-parametrized Conway-Maxwell-Poisson regression models for dispersed counts. Stat. Modelling doi:10.1177/1471082X17697749

G. Shmueli, T. P. Minka, J. B. Kadane, S. Borle and P. Boatwright (2005) A useful distribution for fitting discrete data: revival of the Conway-Maxwell-Poisson distribution. Appl. Statist. 54: 127-142.

Sellers KF, Shmueli G (2010) A Flexible Regression Model for Count Data. Ann. Appl. Stat. 4: 943–961

```
if (spaMM.getOption("example_maxtime")>0.9) {
    # Fitting COMPoisson model with estimated nu parameter:
    #
    data("freight") ## example from Sellers & Shmueli, Ann. Appl. Stat. 4: 943-961 (2010)
    fitme(broken ~ transfers, data=freight, family = COMPoisson())
    fitme(broken ~ transfers, data=freight, family = COMPoisson(link="log"))

# glm(), HLCor() and HLfit() handle spaMM::COMPoisson() with fixed overdispersion:
    #
    glm(broken ~ transfers, data=freight, family = COMPoisson(nu=10))
    HLfit(broken ~ transfers+(1|id), data=freight, family = COMPoisson(nu=10),method="ML")

# Equivalence of poisson() and COMPoisson(nu=1):
    #
    COMPglm <- glm(broken ~ transfers, data=freight, family = poisson())
    coef(COMPglm)</pre>
```

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```
logLik(COMPglm)
COMPglm <- glm(broken ~ transfers, data=freight, family = COMPoisson(nu=1))
coef(COMPglm)
logLik(COMPglm)
HLfit(broken ~ transfers, data=freight, family = COMPoisson(nu=1))
}</pre>
```

composite-ranef

Composite random effects

## **Description**

An example of a composite random effect is corrMatrix(sex|pair). It combines features of a random-coefficient model (sex|pair) and of an autocorrelated random effect corrMatrix(.|.). The random-coefficient model is characterized by a 2\*2 covariance matrix  $\mathbf{C}$  for the random effects  $u_{1,pair}$  and  $u_{2,pair}$  both affecting each of the two sexes for each pair, and the corrMatrix random effect assumes that elements of each of the two vectors  $u_i = (u_{i,pair})$  for pair=1,...,P are correlated according to a given P\*P correlation matrix  $\mathbf{A}$ . Then the composite random effect is defined as the one with 2P\*2P covariance matrix kronecker( $\mathbf{C}$ , $\mathbf{A}$ ).

The definition of composite random effects through the kronecker product may be motivated and understood in light of a quantitative-genetics application (see help("Gryphon") for an example). In this context the two response variables are typically two individual traits. Each trait is affected by two sets of genes, the effect of each set being represented by a gaussian random effect (u\_1 or u\_2). The effect of genetic relatedness on the correlation of random effects u\_i, ID among individuals ID within each set i of genes is described by the corrMatrix  $\mathbf{A}$ . The effects on the two traits for each individual are interpreted as different linear combinations of these two random effects (the coefficients of these linear combinations determining the  $\mathbf{C}$  matrix). Under these assumptions the correlation matrix of the responses (in order (trait, individual)=(1,1)...(1,ID)... (2,1)...(2,ID)...) is indeed kronecker( $\mathbf{C}$ , $\mathbf{A}$ ).

Composite random effects are not restricted to corrMatrix terms, and can also be fitted for multivariate-response models. For example, Matern(mv(1,2)|longitude+latitude) terms can be fitted, in which case the correlation model is still defined through the Kronecker product, where **A** will be a (fitted) Matérn correlation matrix, and **C** will be the correlation matrix of the fitted random-coefficient model for the mv virtual factor for multivariate response.

Implementation and tests of composite random effects is work in progress, with the following ones having been tested: corrMatrix, Matern, Cauchy, adjacency, IMRF, AR1, and to a lesser extent MaternIMRFa. Fits of other composite terms may fail. Even if they succeed, not all post-fit procedures may be operational: in particular, prediction (and then, simulation) with newdata may not yet work. Further, as for random-coefficient terms in univariate-response models, some components of the computed prediction variance depend on a poorly characterized approximation, yielding different results for different fitting algorithms (see Details in predVar).

The summary of the model provides fitted parameters for **A** if this matrix derives from a parametric correlation model (e.g., Matern), and a description of the **C** matrix where it is viewed as a covariance matrix, parametrized by its variances and its correlation coefficient(s). In a standard random-coefficient model these variances would be those of the correlated random effects (see

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summary. HLfit). In the composite random-effect model this is not necessarily so as the variance of the correlated random effects also depend on the variances implied by the A matrix, which are not necessarily 1 if A is a covariance matrix rather than simply a correlation matrix.

A fix>(<LHS>|<RHS>) term is \*not\* a composite random effect when the LHS in boolean, a factor from boolean, or "0+numeric". See the Matérn examples, and the corrMatrix "<LHS> is 0+numeric" example, below.

```
if (spaMM.getOption("example_maxtime")>1.8) {
#### corrMatrix examples
############################
## Toy data preparation
data("blackcap")
toy <- blackcap
toySID \leftarrow gl(7,2)
grp < - rep(1:2,7)
toy$migStatus <- toy$migStatus +(grp==2)</pre>
toy$loc <- rownames(toy) # to use as levels matching the corrMatrix dimnames
toy$grp <- factor(grp)</pre>
toy$bool <- toy$grp==1L
toy$boolfac <- factor(toy$bool)</pre>
toy$num <- seq(from=1, to=2, length.out=14)
## Build a toy corrMatrix as perturbation of identity matrix:
n_rhs <- 14L
eps <- 0.1
set.seed(123)
rcov <- ((1-eps)*diag(n_rhs)+eps*rWishart(1,n_rhs,diag(n_rhs)/n_rhs)[,,1])</pre>
# eigen(rcov)$values
colnames(rcov) <- rownames(rcov) <- toy$loc # DON'T FORGET NAMES</pre>
##### Illustrating the different LHS types
### <LHS> is logical (TRUE/FALSE) => No induced random-coefficient C matrix;
   corrMatrix affects only responses for which <LHS> is TRUE:
(fit1 <- fitme(migStatus ~ bool + corrMatrix(bool|loc), data=toy, corrMatrix=rcov))</pre>
# Matrix::image(get_ZALMatrix(fit1))
### <RHS> is a factor built from a logical => same a 'logical' case above:
(fit2 <- fitme(migStatus ~ boolfac + corrMatrix(boolfac|loc), data=toy, corrMatrix=rcov))</pre>
```

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```
# Matrix::image(get_ZALMatrix(fit2))
### <RHS> is a factor not built from a logical:
# (grp|.) and (0+grp|.) lead to equivalent fits of the same composite model,
   but contrasts are not used in the second case and the C matrices differ,
   as for standard random-coefficient models.
(fit1 <- fitme(migStatus ~ grp + corrMatrix(grp|loc), data=toy, corrMatrix=rcov))</pre>
(fit2 <- fitme(migStatus ~ grp + corrMatrix(0+grp|loc), data=toy, corrMatrix=rcov))</pre>
# => same fits, but different internal structures:
Matrix::image(fit1$ZAlist[[1]]) # (contrasts used)
Matrix::image(fit2$ZAlist[[1]]) # (contrasts not used)
# Also compare ranef(fit1) versus ranef(fit2)
#
## One can fix the C matrix, as for standard random-coefficient terms
(fit1 <- fitme(migStatus ~ grp + corrMatrix(0+grp|loc),data=toy, corrMatrix=rcov,</pre>
               fixed=list(ranCoefs=list("1"=c(1,0.5,1))))
# same result without contrasts hence different 'ranCoefs':
(fit2 <- fitme(migStatus ~ grp + corrMatrix(grp|loc), data=toy, corrMatrix=rcov,
               fixed=list(ranCoefs=list("1"=c(1,-0.5,1))))
### <LHS> is numeric (but not '0+numeric'):
# composite model with C being 2*2 for Intercept and numeric variable
(fitme(migStatus ~ num + corrMatrix(num|loc), data=toy, corrMatrix=rcov))
### <LHS> is 0+numeric: no random-coefficient C matrix
# as the Intercept is removed, but the correlated random effects
# arising from the corrMatrix are multiplied by sqrt(<numeric variable>)
(fitme(migStatus ~ num + corrMatrix(0+num|loc), data=toy, corrMatrix=rcov))
### <LHS> for multivariate response (see help("Gryphon") for more typical example)
## More toy data preparation for multivariate response
ch <- chol(rcov)</pre>
set.seed(123)
v1 <- tcrossprod(ch,t(rnorm(14,sd=1)))</pre>
v2 <- tcrossprod(ch,t(rnorm(14,sd=1)))</pre>
toy$status <- 2*v1+v2
toy$status2 <- 2*v1-v2
## Fit·
fitmv(submodels=list(mod1=list(status ~ 1+ corrMatrix(0+mv(1,2)|loc)),
                     mod2=list(status2 ~ 1+ corrMatrix(0+mv(1,2)|loc))),
      data=toy, corrMatrix=rcov)
```

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```
#### Matern examples: sex-dependent random effects
if (spaMM.getOption("example_maxtime")>2) {
data(Leuca)
subLeuca <- Leuca[c(1:10,79:88),] # subset for faster examples</pre>
# The random effects in the following examples are composite because 'sex' is not
\# boolean nor factor from boolean. If 'Matern(factor(female)|x+y)' were used, the effect
# would be the same 'Matern(female|x)', fitting
 fitme(fec_div ~ 1 + Matern(sex|x+y),data=subLeuca) # => builds a random effect
# correlated across sexes, from 2 independent realizations u_1 and u_2 of 20 values
# (for the 20 locations in the data). In a (sex|x) term the 20 values would be
# independent from each other within each u_i. In the Matern(sex|x+y) such 20 values
# are autocorrelated within each u_i.
# For pedagogic purposes, one can also fit
 fitme(fec_div ~ 1 + Matern(sex|x + y %in% sex),data=subLeuca)
# which again builds a random effect from 2 independent realizations
# u_1 and u_2, but each u_i now contains two realizations u_i1 and u_i2 of 10 values,
# autocorrelated within each u_ij following the Matern model,
# but independent between u_i1 and u_i2. As a result, the overall random effect in each sex,
# v_m or v_f, is a weighted sum of two sex-specific Matern random effect,
# so that v_m and v_f are independent from each other.
}
}
```

confint.HLfit

Confidence intervals

# Description

This function interfaces two procedures: a profile confidence interval procedure implemented for fixed-effects coefficients only; and a parametric bootstrap procedure that can be used to provide confidence interval for any parameter, whether a canonical parameter of the model or any function of one or several such parameters. The bootstrap is performed if the parm argument is a function or a quoted expression or if the boot\_args argument is a list. The profile confidence interval is computed if neither of these conditions is true. In that case parm must be the name(s) of some **fixed-effect** coefficient, and the (p\_v approximation of the) profile likelihood ratio for the given parameter is used to define the interval, where the profiling is over all other fitted parameters, including other fixed-effects coefficients, as well as variances of random effects and spatial correlations if these were fitted.

Of related interest, see numInfo which evaluates numerically the information matrix for given sets of canonical model parameters, from which asymptotic confidence intervals can be deduced.

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### Usage

#### **Arguments**

object An object of class HLfit, as returned by the fitting functions in spaMM.

parm character vector, integer vector, or function, or a quoted expression. If char-

acter, the name(s) of parameter(s) to be fitted; if **integer**, their position in the fixef(object) vector. Valid names are those of this vector. If a **function**, it must return a (vector of) parameter estimate(s) from a fit object. If a **quoted** expression, it must likewise extract parameter estimate(s) from a fit object; this

expression must refer to the fitted object as 'hlfit' (see Examples).

level The coverage of the interval.

verbose whether to print the interval or not. As the function returns its more extensive

results invisibly, this printing is the only visible output.

boot\_args NULL or a list of arguments passed to functions spaMM\_boot and boot.ci. It

must contain element nsim (for spaMM\_boot). The type argument of boot.ci can only be given as element ci\_type, to avoid conflict with the type argument

of spaMM\_boot.

format Only effective non-default value is "stats" to return results in the format of the

stats::confint result (see Value).

... Additional arguments (maybe not used, but conforming to the generic definition

of confint).

#### Value

The format of the value varies, but in all cases distinguished below, one or more tables are included, as a table attribute, in the format of the stats::confint result, to facilitate consistent extraction of results. By default confint returns invisibly the full values described below, but if format="stats", only the table attribute is returned.

If a profile CI has been computed for a single parameter, a list is returned including the confidence interval as shown by verbose=TRUE, and the fits lowerfit and upperfit giving the profile fits at the confidence bounds. This list bears the table attribute.

If a profile CI has been computed for several parameters, a structured list, named according to the parameter names, of such single-parameter results is returned, and a single table attribute for all parameters is attached to the upper level of the list.

If a bootstrap was performed, for a single parameter the result of the boot.ci call is returned, to which a table attribute is added. This table is now a list of tables for the different bootstrap CI types (default being normal, percent, and basic), each such table in the format of the stats::confint results. For several parameters, a named list of boot.ci results is returned, its names being the parameter names, and the table attribute is attached to the upper level of the list.

The boot.ci return value for each parameter includes the call to boot.ci. This call is typically shown including a long t vector, which makes a bulky display. spaMM hacks the printing to abbreviate long ts.

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#### See Also

numInfo for information matrix.

#### **Examples**

```
data("wafers")
wfit <- HLfit(y ~X1+(1|batch), family=Gamma(log), data=wafers, method="ML")
confint(wfit,"X1") # profile CI
if (spaMM.getOption("example_maxtime")>30) {
   # bootstrap CI induced by 'boot_args':
  confint(wfit,names(fixef(wfit)), boot_args=list(nsim=99, seed=123))
   # bootstrap CI induced by 'parm' being a function:
  confint(wfit,parm=function(v) fixef(v),
           boot_args=list(nb_cores=10, nsim=199, seed=123))
  # Same effect if 'parm' is a quoted expression in terms of 'hlfit':
  confint(wfit,parm=quote(fixef(hlfit)),
           boot_args=list(nb_cores=10, nsim=199, seed=123))
   # CI for the variance of the random effect:
   ci <- confint(wfit,parm=function(fit){get_ranPars(fit)$lambda[1]},</pre>
        boot_args=list(nb_cores=10, nsim=199, seed=123))
   # The distribution of bootstrap replicates:
  plot(ecdf(ci$call$t))
   # We may be far from ideal condition for accuracy of bootstrap intervals;
   # for variances, a log transformation may sometimes help, but not here.
  # Passing arguments to child processes, as documented in help("spaMM_boot"):
  set.seed(123)
  rvar <- runif(nrow(wafers))</pre>
  wrfit <- fitme(y ~X1+(1|batch), family=Gamma(log), data=wafers, fixed=list(phi=rvar))</pre>
   confint(wrfit, parm = "(Intercept)", boot_args = list(nsim = 100, nb_cores = 2,
           fit_env = list(rvar=rvar)))
}
```

control.HLfit

Control parameters of the HLfit fitting algorithm

#### **Description**

A list of parameters controlling the HLfit fitting algorithm (potentially called by all fitting functions in **spaMM**), which should mostly be ignored in routine use. Possible controls are:

```
algebra, sparse_precision: see algebra;
```

conv.threshold and spaMM\_tol: spaMM\_tol is a list of tolerance values, with elements Xtol\_rel and Xtol\_abs that define thresholds for relative and absolute changes in parameter values in iterative algorithms (used in tests of the form "d(param)< Xtol\_rel \* param + Xtol\_abs", so that

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Xtol\_abs is operative only for small parameter values). conv.threshold is the older way to control Xtol\_rel. Default values are given by spaMM.getOption("spaMM\_tol");

break\_conv\_logL: a boolean specifying whether the iterative algorithm should terminate when log-likelihood appears to have converged (roughly, when its relative variation over on iteration is lower than 1e-8). Default is FALSE (convergence is then assessed on the parameter estimates rather than on log-likelihood).

iter.mean.dispFix: the number of iterations of the iterative algorithm for coefficients of the linear predictor, if no dispersion parameters are estimated by the iterative algorithm. Defaults to 200 except for Gamma(log)-family models;

iter.mean.dispVar: the number of iterations of the iterative algorithm for coefficients of the linear predictor, if some dispersion parameter(s) is estimated by the iterative algorithm. Defaults to 50 except for Gamma(log)-family models;

max.iter: the number of iterations of the iterative algorithm for joint estimation of dispersion parameters and of coefficients of the linear predictor. Defaults to 200. This is typically much more than necessary, unless there is little information to separately estimate  $\lambda$  and  $\phi$  parameters;

resid.family: was a previously documented control (before version 2.6.40), and will still operate as previously documented, but should not be used in new code.

# Usage

```
# <fitting function>(., control.HLfit=list(...))
```

convergence

Assessing convergence for fitted models

# **Description**

spaMM fits can produce various convergence warnings or messages.

Messages referring to convergence issues in initialization can generally be ignored but may help to diagnose other apparent problems, if any.

Warnings referring to  $.calc\_dispGammaGLM$  (for residual-dispersion fits) can generally be ignored when they show a small criterion (say <1e-5) but may otherwise suggest that the final fit did not optimize its objective.

Messages pointing to slow convergence and drawing users to this doscumentation do not necessarily mean the fit is incorrect. Rather, they suggest that another fitting strategy could be tried. Keep in mind that several parameters (notably the dispersion parameters: the variance of random effects and the residual variance parameter, if any) can be estimated either by the iterative algorithms, or by generic optimization methods. In my experience, slow convergence happens in certain cases where a large random-effect variance is considered by the algorithm used.

How to know which algorithm has been selected for each parameter? fitme(., verbose=c(TRACE=TRUE)) shows successive values of the variables estimated by optimization (See Examples; if no value appears, then all are estimated by iterative methods). The first lines of the summary of a fit object should tell which variances are estimated by the "outer" method.

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If the iterative algorithm is being used, then it is worth trying to use the generic optimization methods. In particular, if you used HLfit, try using fitme; if you already use fitme, try to enforce generic optimization of the random-effect variance(s) (see inits). Conversely, if generic optimization is being used, the maximum lambda value could be controlled (say, upper=list(lambda=c(10,NA))), or the iterative algorithm can be called (see inits again).

For the largest datasets, it may be worth comparing the speed of the "spcorr" and "spprec" choices of the algebra control, in case spaMM has not selected the most appropriate by default. However, this will not be useful for geostatistical models with many spatial locations.

# **Examples**

# See help("inits") for examples of control by initial values.

corMatern

Matern Correlation Structure as a corSpatial object

# **Description**

This implements the Matérn correlation structure (see Matern) for use with 1me or g1mmPQL. Usage is as for others corSpatial objects such as corGaus or corExp, except that the Matérn family has an additional parameter. This function was defined for comparing results obtained with corrHLfit to those produced by 1me and g1mmmPQL. There are problems in fitting (G)LMMs in the latter way, so it is not a recommended practice.

# Usage

```
corMatern(value = c(1, 0.5), form = ~1, nugget = FALSE, nuScaled = FALSE,
    metric = c("euclidean", "maximum", "manhattan"), fixed = FALSE)
```

# Arguments

value

An optional vector of parameter values, with serves as initial values or as fixed values depending on the fixed argument. It has either two or three elements, depending on the nugget argument.

If nugget is FALSE, value should have two elements, corresponding to the "range" and the "smoothness"  $\nu$  of the Matérn correlation structure. If value has zero length, the default is a range of 90% of the minimum distance and a smoothness of 0.5 (exponential correlation). Warning: the range parameter used in corSpatial objects is the inverse of the scale parameter used in MaternCorr and thus they have opposite meaning despite both being denoted  $\rho$  elsewhere in this package or in nlme literature.

If nugget is TRUE, meaning that a nugget effect is present, value can contain two or three elements, the first two as above, the third being the "nugget effect" (one minus the correlation between two observations taken arbitrarily close together). If value has length zero or two, the nugget defaults to 0.1. The range and smoothness must be greater than zero and the nugget must be between zero and one.

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form (Pasted from corSpatial) a one sided formula of the form ~ S1+...+Sp, or ~

S1+...+Sp | g, specifying spatial covariates S1 through Sp and, optionally, a grouping factor g. When a grouping factor is present in form, the correlation structure is assumed to apply only to observations within the same grouping level; observations with different grouping levels are assumed to be uncorrelated. Defaults to  $\sim$  1, which corresponds to using the order of the observations

in the data as a covariate, and no groups.

nugget an optional logical value indicating whether a nugget effect is present. Defaults

to FALSE.

nuScaled If nuScaled is set to TRUE the "range" parameter  $\rho$  is divided by  $2\sqrt{\nu}$ . With

this option and for large values of  $\nu$ , corMatern reproduces the calculation of corGaus. Defaults to FALSE, in which case the function compares to corGaus

with range parameter  $2(\sqrt{\nu})\rho$  when  $\nu$  is large.

metric (Pasted from corSpatial) an optional character string specifying the distance

metric to be used. The currently available options are "euclidean" for the root sum-of-squares of distances; "maximum" for the maximum difference; and "manhattan" for the sum of the absolute differences. Partial matching of arguments is used, so only the first three characters need to be provided. Defaults to

"euclidean".

fixed an optional logical value indicating whether the coefficients should be allowed

to vary in the optimization, or kept fixed at their initial value. Defaults to FALSE,

in which case the coefficients are allowed to vary.

# **Details**

This function is a constructor for the corMatern class, representing a Matérn spatial correlation structure. See MaternCorr for details on the Matérn family.

# Value

an object of class corMatern, also inheriting from class corSpatial, representing a Matérn spatial correlation structure.

# Note

The R and C code for the methods for corMatern objects builds on code for corSpatial objects, by D.M. Bates, J.C. Pinheiro and S. DebRoy, in a circa-2012 version of nlme.

#### References

Mixed-Effects Models in S and S-PLUS, José C. Pinheiro and Douglas M. Bates, Statistics and Computing Series, Springer-Verlag, New York, NY, 2000.

#### See Also

glmmPQL, 1me

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# **Examples**

```
## LMM
data("blackcap")
blackcapD <- cbind(blackcap,dummy=1) ## obscure, isn't it?</pre>
## With method= 'ML' in lme, The correlated random effect is described
## as a correlated residual error and no extra residual variance is fitted:
nlme::lme(fixed = migStatus ~ means, data = blackcapD, random = ~ 1 | dummy,
    correlation = corMatern(form = ~ longitude+latitude | dummy),
    method = "ML", control=nlme::lmeControl(sing.tol=1e-20))
## Binomial GLMM
if (spaMM.getOption("example_maxtime")>32) {
 data("Loaloa")
 LoaloaD <- cbind(Loaloa,dummy=1)</pre>
 MASS::glmmPQL(fixed =cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI,
        data = LoaloaD, random = ~ 1 | dummy, family=binomial,
        correlation = corMatern(form = ~ longitude+latitude | dummy))
}
```

corrFamily

Using corrFamily constructors and descriptors.

## **Description**

One can declare and fit correlated random effects belonging to a user-defined correlation (or covariance) model (i.e., a parametric family of correlation matrices, although degenerate case with no parameter are also possible). This documentation is a first introduction to this feature. It is experimental in the sense that its design has been formalized only from a limited number of corrFamily examples, and that the documentation is not mature. Implementing prediction for random-effects defined in this way may be tricky. A distinct documentation corrFamily-design provides more information for the efficient design of new correlation models to be fitted in this way.

A simple example of random-effect model implemented in this way is the autoregressive model of order p (AR(p) in the literature; specifically documented elsewhere, see ARp). It can be used as a formula term like other autocorrelated random-effects predefined in **spaMM**, to be fitted by fitme or fitmv:

```
fitme(lh ~ 1 + ARp(1|time, p=3), # <= declaration of random effect
  < data and other possible arguments >)
```

User-defined correlation models should be registered for this simple syntax to work (see Details for an alternative syntax):

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The ARp object here copied in myARp is a function (the *corrFamily constructor*) which returns a list (the *corrFamily descriptor*) which contains the necessary information to fit a random effect with an AR(p) correlation. The p argument in the myARp(1|time, p=3) term enforces evaluation of myARp(p=3), producing the descriptor for the AR(3) model. The structure of this descriptor is

```
List of 5
               :function (parvec)
$ Cf
 ..- < with some attribute >
$ tpar : num [1:3] 0.5 0.333 0.25
$ type
            : chr "precision"
$ initialize :function (Zmatrix, ...)
  ..- < with some attribute >
           : NULL
$ fixed
$ calc_moreargs:function (corrfamily, ...)
  ..- < with some attribute >
              : chr "time_series"
$ levels_type
$ calc_corr_from_dist:function (ranFix, char_rd, distmat, ...)
  ..- < with some attribute >
 < and possibly other elements >
```

The meaning of these elements and some additional ones is explained below.

Only Cf and tpar are necessary elements of a corrFamily object. If one designs a new descriptor where some other elements are absent, **spaMM** will try to provide plausible defaults for these elements. Further, if the descriptor does not provide parameter names (as the names of tpar, or in some more cryptic way), default names "p1", "p2"... will be provided.

# Usage

```
## corrFamily descriptor provided as a list of the form
#
# list(Cf=<.>, tpar=<.>, ...)

## corrFamily constructor: any function that returns
# a valid corrFamily descriptor
#
# function(tpar=<.>, fixed=<.>, ...) # typical but not mandatory arguments
## There is a distinct documentation page for 'register_cF'.
```

# **Arguments**

# **Elements** of the corrFamily descriptor:

Cf	(required): function returning the correlation matrix (or covariance matrix, or their inverse), given its first argument, a parameter vector.
tpar	(required): a feasible argument of Cf. tpar is <b>not</b> an initial <b>nor</b> a fixed value.
type	optional, but required if the return value of Cf is an inverse correlation matrix rather than a correlation matrix, in which case one should specify type="precision".

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fixed optional: fixed values for some correlation parameters, provided as a named

vector with names consistent with those to be used for tpar. This is conceived to achieve the same statistical fit as by using the fixed argument of fitme, although the structure of the result of the fit differs in some subtle ways whether parameters are fixed through the descriptor or through the fitting function (see

Examples in ARp).

calc\_moreargs optional: a function returning a list with possible elements init, lower and

upper for control of estimation (and possibly other elements for other purposes). If the descriptor does not provide this function, a default calc\_moreargs will

be provided, implementing unbounded optimization.

initialize optional: a function evaluating variables that may be needed repeatedly by Cf or

Af.

Af This function should be defined if the correlation model requires an **A** matrix

(the middle term in the case the design matrix of a random effect term is described by a triple matrix product **ZAL** as described in random-effects). Examples can be found in the descriptors returned by the ranGCA and MaternIMRFa

constructors.

levels\_type In the above example its value "time\_series" informs **spaMM** that levels of

the random effect should be considered for all integer values within the range of the time variable, not only for levels present in the data. If this element is not provided by the constructor, **spaMM** will internally assume a levels\_type suitable for geostatistical models. Further level types may be defined in the

future.

calc\_corr\_from\_dist, make\_new\_corr\_lists

Functions possibly needed for prediction (see Details).

need\_Cnn optional: a boolean; default is TRUE. Controls prediction computations (see

Details).

public An environment where some variables can be saved, typically by the initialize

expression, for inspection at user level and for re-use. See diallel for an ex-

ample.

#### *fitting-function* arguments:

lower, upper, init and fixed optimization controls can be used to control optimization of continuous parameters as for other random-effect parameters. They are specified as numeric vectors, themselves being element of the corrPars list (see Examples in corrFamily-design). Parameter names (consistent with those to be used for the tpar argument) may be required to disambiguate incomplete vectors (e.g., to specify only its second element). Apart from fixed ones, any of the values not specified through the fitting-function arguments will be sought in the return value of the calc\_moreargs function, if provided in the descriptor. If the lower or upper information is missing there, it must be provided throught the fitting-function call. If the init information is missing, a default value will be deduced from the bounds. The init specification is thus always optional while the bounds specification is optional only if the descriptor provides default values.

# Arguments of the corrFamily constructor

These may be ad libitum, as design rules are defined only for the returned descriptor. However, arguments tpar, fixed, and public of predefined constructors, such as ARp, are designed to match the above respective elements of the descriptor.

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#### **Details**

#### \* Constructor elements for prediction:

For prediction of autocorrelated random effects, one must first assess whether levels of the random effect not represented in the fit are possible in new data (corresponding to new spatial locations in geostatistical models, or new time steps in time series). In that case need\_Cnn must be TRUE (Interpolated MRFs do not require this as all required random-effect levels are determined by the IMRF mesh argument rather than by the fitted data or new data).

Next, for autocorrelated random effects where need\_Cnn is TRUE, a make\_new\_corr\_lists function must be provided, except when a calc\_corr\_from\_dist function is instead provided (which may be sufficient for models that construct the correlation from a spatial distance matrix). When need\_Cnn is FALSE, a make\_new\_corr\_lists function may still be needed.

The Examples section provides a simple example of such design, and the source code of the ARp or ARMA constructors provide further examples. They show that the make\_new\_corr\_lists function may assign matrices or vectors as elements of several lists contained in a newLv\_env environment. A matrix is assigned in the cov\_newLv\_oldv\_list, specifying correlations between "new" levels of the random effect (implied by the new data) and "old" levels (those already included in the design matrix of the random effect for the fit). If need\_Cnn is TRUE, a second matrix may be assigned in the cov\_newLv\_newLv\_list, specifying correlation between "new" levels, and the diagonal of this matrix is assigned in the diag\_cov\_newLv\_newLv\_list. The overall structure of the code (the conditions where these assignments are performed, and the list indices), should be conserved.

When calling simulate(., newdata=<non-NULL>, type="marginal", a fourth matrix may be useful, assigned into a L\_newLv\_newLv\_list, specifying the matrix root (as a tcrossprod factor) of the correlation matrix stored in cov\_newLv\_newLv\_list. The relevant **spaMM** procedure will however try to compute it on the fly when it has not been provided by the make\_new\_corr\_lists function.

### \* Fitting a corrFamily without a constructor:

It is possible to use an unregistered corrFamily, as follows:

```
AR3 <- ARp(p=3)  # Generate descriptor of AR model of order 3
fitme(lh ~ 1 + corrFamily(1|time), # <= declaration of random effect
  covStruct=list(
    corrFamily= AR3  # <= declaration of its correlation structure
  ),
  < data and other possible arguments >)
```

Here the fit only uses a descriptor list, not a constructor function. This descriptor is here provided to the fitting function as an element of the covStruct argument (using the general syntax of this argument), and in the model formula the corresponding random effect is declared as a term of the form

```
corrFamily(1|<grouping factor>).
```

This syntax is more complex than the one using a registered constructor, but it might be useful for development purposes (one only has to code the descriptor, not the constructor function). However, it is not general; in particular, using registered constructors may be required to obtain correct results when fitting multivariate-response models by fitmv.

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#### See Also

See ARp, diallel, and MaternIMRFa for basic examples of using a predefined corrFamily descriptor, and corrFamily-design for more geeky stuff including examples of implementing simple new correlation families.

```
## Not run:
### Minimal (with many features missing) reimplementation
      of corrMatrix() terms as a corrFamily
corrMatrix_cF <- function(corrMatrix) {</pre>
 force(corrMatrix) # Makes it available in the environment of the functions next defined.
 oldZlevels <- NULL
 initialize <- function(Zmatrix, ...) {</pre>
  oldZlevels <<- colnames(Zmatrix) # Pass info about levels of the random effect in the data.
 Cf <- function(newlevels=oldZlevels ) {</pre>
    if (length(newlevels)) {
      corrMatrix[newlevels, newlevels]
    } else corrMatrix[oldZlevels,oldZlevels] # for Cf(tpar=numeric(0L))
 }
 calc_moreargs <- function(corrfamily, ...) {</pre>
    list(init=c(),lower=c(),upper=c())
 }
 make_new_corr_lists <- function(newLv_env, which_mats, newZAlist, new_rd, ...) {</pre>
    newlevels <- colnames(newZAlist[[new_rd]])</pre>
  newLv_env$cov_newLv_oldv_list[[new_rd]] <- corrMatrix[newlevels,oldZlevels, drop=FALSE]</pre>
    if (which_mats$nn[new_rd]) {
    newLv_env$cov_newLv_newLv_list[[new_rd]] <- corrMatrix[newlevels, newlevels, drop=FALSE]</pre>
   } else {
      newLv_env$diag_cov_newLv_newLv_list[[new_rd]] <- rep(1,length(newlevels))</pre>
 }
 list(Cf=Cf, tpar=numeric(0L), initialize=initialize, calc_moreargs=calc_moreargs,
       make_new_corr_lists=make_new_corr_lists,
       tag="corrMatrix_cF")
}
register_cF("corrMatrix_cF")
# usage:
data("blackcap")
MLcorMat <- MaternCorr(proxy::dist(blackcap[,c("latitude","longitude")]),</pre>
```

### **Description**

Tentative formal rules for definition of corrFamily descriptors (work in progress). This is likely to repeat and extend information partially given in corrFamily and corrFamily-design documentations.

User-level rules (not relevant fo corrFamily descriptors internally modified during a fit):

- tpar Should always be present. For trivial parameterless cases (e.g. ranGCA), it should be numeric(0L), not NULL.
- **Cf** function; should always be present. For trivial uncorrelated random effects (e.g. ranGCA, where only the Af function carries the information for the model), it should return an identity matrix, not NULL, with row names to be matched to the column names of the **Z** matrix for the random effect.
- **calc\_moreargs** optional function. If present, it should have formal arguments including at least corrfamily and ....
- **Af** function; optional. If present, it should have row names to be matched to the column names of the **Z** matrix for the random effect, and also needs column names if it is to be matched with the row names of a correlation matrix (or its inverse).
- initialize Optional function. If present, should have formal arguments including at least Zmatrix
  and ....
  - In predefined corrFamily constructors, variables created by initialize for use by Cf or Af should be declared (typically as NULL) in the body of the constructor, so that R CMD check does not complain.
- **public** An environment. initialize may write into it. It might also read into it, for example read the result of a long previous computation by initialize during a previous fit, though this opens the door to various errors.

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corrFamily-design	Designing new corrFamily descriptors for parametric correlation families
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### **Description**

This documentation describe additional design features to be taken into account when defining a new corrFamily descriptor for a correlation model. Using such a descriptor will be more efficient than the equally general method, of maximizing an objective function of the correlation parameters that calls (say) fitme() on a model including a corrMatrix itself function of the correlation parameters. But this may still be inefficient if a few issues are ignored.

### For elements of the corrFamily descriptor for basic cases:

- Cf The function value should (1) be of constant class for all parameter values. For families of mathematically sparse matrices, the CsparseMatrix class is recommended (and more specifically the dsCMatrix class since the matrix is symmetric); (2) have row names that match the levels of the grouping factor (the nested random effect Example shows the code needed when this nested effect is defined from two variables).
- tpar In order to favor the automatic selection of suitable algorithms, tpar should be chosen so that Cf(tpar) is **least** sparse (i.e., has the minimal number of elements equal to zero) in the correlation family, in terms of its sparsity and of the sparsity of its inverse. A tpar yielding an identity matrix is often a \*bad\* template as least sparse correlation matrices and their inverses are denser for most families except diagonal ones. For degerate corrFamily objects that describe a constant correlation model rather than a parametric family, use tpar=numeric(0).
- **type** Do not forget type="precision" it if the return value of Cf is an inverse correlation matrix rather than a correlation matrix, in which case one should specify.
- **calc\_moreargs** should have formal arguments including at least corrfamily and . . . . The source code of ARp, ARMA or diallel shows the expected structure of its return value.

### For advanced features of the corrFamily descriptor:

- Af Af has (minimally) three formal arguments (newdata, term, ...). spaMM will call Af with distinct values of the newdata argument for the fit, and for predictions for new data. For the curious: the term argument that will be provided by spaMM to Af is the formula term for the random effect an object of class call, as obtained e.g. by
  - (~1+ corrFamily(1 | longitude + latitude))[[2]][[3]] —, which will provide the names of the variables that need to be taken from the newdata to construct the matrix returned by Af.

#### **Details**

• **spaMM** will regularize invalid or nearly-singular correlation or covariance matrices internally if the correlation function has not done so already, but it it better to control this in the correlation function. The **regularize** convenience function is available for that purpose, but parametrizations that avoid the need for regularization are even better, since fitting models with nearly-singular correlation matrices is prone to various difficulties (The Toeplitz example below is good to illustrate potential problems but is otherwise poor as it produces non-positive definite matrices; the ARP constructor illustrates a parametrization that avoids that problem).

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• Users should make sure that any regularized matrix still belongs to the intended parametric family of matrices, and they should keep in mind that the **spaMM** output will show the input parameters of the unregularized matrix, not the parameters of the regularized one (e.g., in the Toeplitz example below, the fitted matrix is a regularized Toepliz matrix with slightly different coefficients than the input parameters).

And for efficiency,

- Let us repeat that the correlation function should return matrices of constant class, and in sparse format when the matrices are indeed mathematically sparse. For mathematically dense matrices (as in the Toeplitz example below), the dsyMatrix class may be suitable.
- Let us repeat that in order to favor the automatic selection of suitable algorithms, tpar should be chosen so that Cf(tpar) is **least** sparse in the correlation family. For matrices of CsparseMatrix, a check is implemented to catch wrong choices of tpar.
- For challenging problems (large data, many parameters...) it may pay to optimize a bit the correlation function. The Example of nested effects with heterogenous variance below illustrates a possible trick. In the same cases, It may also pay to try the alternative algebraic methods, by first comparing speed of the different methods (control.HLfit=list(algebra=<"spprec"|"spcorr"|"decorr">)) for given correlation parameter values, rather than to assume that spaMM will find the best method (even if it often does so).
- The corrFamily descriptor may optionally contain booleans possiblyDenseCorr and sparsePrec to help spaMM select the most appropriate matrix algebraic methods. sparsePrec should be set to TRUE if sparse-precision methods are expected to be efficient for fitting the random effect. possiblyDenseCorr should be set to FALSE if the correlation matrix is expected to be sparse, which means here that less than 15% of its elements are non-zero.

```
if (spaMM.getOption("example_maxtime")>2 &&
      requireNamespace("agridat", quietly = TRUE)) {
data("onofri.winterwheat", package="agridat")
##### Fitting a Toeplitz correlation model for temporal correlations #####
# A Toeplitz correlation matrix of dimension d*d has d-1 parameters
# (by symmetry, and with 1s on the main diagonal). These d-1 parameters
# can be fitted as follows:
Toepfn <- function(v) {</pre>
 toepmat <- Matrix::forceSymmetric(toeplitz(c(1,v))) # dsyMatrix</pre>
 # Many of the matrices in this family are not valid correlation matrices;
     the regularize() function is handy here:
 toepmat <- regularize(toepmat, maxcondnum=1e12)</pre>
 # And don't forget the rownames!
 rownames(toepmat) <- unique(onofri.winterwheat$year)</pre>
 toepmat
}
(Toepfit <- spaMM::fitme(</pre>
 yield ~ gen + corrFamily(1|year), data=onofri.winterwheat, method="REML",
```

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```
covStruct=list(corrFamily=list(Cf=Toepfn, tpar=rep(1e-4,6))),
         # (Note the gentle warning if one instead uses tpar=rep(0,6) here)
 lower=list(corrPars=list("1"=rep(-0.999,6))),
 upper=list(corrPars=list("1"=rep(0.999,6)))))
# The fitted matrix is (nearly) singular, and was regularized:
eigen(Corr(Toepfit)[[1]])$values
# which means that the returned likelihood may be inaccurate,
# and also that the actual matrix elements differ from input parameters:
Corr(Toepfit)[[1]][1,-1]
### The usual rules for specifying covStruct, 'lower', 'upper' and 'init' apply
# here when the corrFamily term is the second random-effect:
(Toep2 <- spaMM::fitme(</pre>
       yield ~ 1 + (1|gen) + corrFamily(1|year), data=onofri.winterwheat, method="REML",
        covStruct=list("1"=NULL, corrFamily=list(Cf=Toepfn, tpar=rep(1e-4,6))),
        , init=list(corrPars=list("2"=rep(0.1,6))),
        lower=list(corrPars=list("2"=rep(-0.999,6))),
        upper=list(corrPars=list("2"=rep(0.999,6)))))
##### Fitting one variance among years per each of 8 genotypes. #####
# First, note that this can be *more efficiently* fitted by another syntax:
### Fit as a constrained random-coefficient model:
# Diagonal matrix of NA's, represented as vector for its lower triangle:
ranCoefs_for_diag <- function(nlevels) {</pre>
 vec <- rep(0,nlevels*(nlevels+1L)/2L)</pre>
 vec[cumsum(c(1L,rev(seq(nlevels-1L)+1L)))] <- NA</pre>
 vec
}
(by_rC <- spaMM::fitme(yield ~ 1 + (0+gen|year), data=onofri.winterwheat, method="REML",
                       fixed=list(ranCoefs=list("1"=ranCoefs_for_diag(8)))))
### Fit as a corrFamily model:
gy_levels <- paste0(gl(8,1,length =56,labels=levels(onofri.winterwheat$gen)),":",</pre>
                        gl(7,8,labels=unique(onofri.winterwheat$year)))
# A log scale is often suitable for variances, hence is used below;
# a correct but crude implementation of the model is
diagf <- function(logvar) {</pre>
 corr_map <- kronecker(Matrix::.symDiagonal(n=7),diag(x=exp(logvar)))</pre>
 rownames(corr_map) <- gy_levels</pre>
 corr_map
}
```

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```
# but we can minimize matrix operations as follows:
corr_map <- Matrix::.symDiagonal(n=8,x=seq(8))</pre>
rownames(corr_map) <- unique(onofri.winterwheat$gen)</pre>
diagf <- function(logvar) {</pre>
 corr_map@x <- exp(logvar)[corr_map@x]</pre>
 corr_map
}
                  # (and this returns a dsCMatrix)
(by_cF <- spaMM::fitme(</pre>
        yield ~ 1 + corrFamily(1|gen %in% year), data=onofri.winterwheat, method="REML",
        covStruct=list(corrFamily = list(Cf=diagf, tpar=rep(1,8))),
        fixed=list(lambda=1),
                                          # Don't forget to fix this redundant parameter!
        # init=list(corrPars=list("1"=rep(log(0.1),8))), # 'init' optional
        lower=list(corrPars=list("1"=rep(log(1e-6),8))), \ \# \ 'lower' \ and \ 'upper' \ required
        upper=list(corrPars=list("1"=rep(log(1e6),8)))))
# => The 'gen' effect is nested in the 'year' effect and this must be specified in the
# right-hand side of corrFamily(1|gen %in% year) so that the design matrix 'Z' for the
# random effects to have the correct structure. And then, as for other correlation
# structures (say Matern) it should be necessary to specify only the correlation matrix
# for a given year, as done above. Should this fail, it is also possible to specify the
# correlation matrix over years, as done below. spaMM will automatically detect, from
# its size matching the number of columns of Z, that it must be the matrix over years.
corr_map <- Matrix::forceSymmetric(kronecker(Matrix::.symDiagonal(n=7),diag(x=seq(8))))</pre>
rownames(corr_map) <- gy_levels</pre>
diagf <- function(logvar) {</pre>
 corr_map@x <- exp(logvar)[corr_map@x]</pre>
 corr_map
}
                  # (and this returns a dsCMatrix)
(by_cF <- spaMM::fitme(</pre>
 yield ~ 1 + corrFamily(1|gen %in% year), data=onofri.winterwheat, method="REML",
 covStruct=list(corrFamily = list(Cf=diagf, tpar=rep(1,8))),
 fixed=list(lambda=1),
                                    # Don't forget to fix this redundant parameter!
 # init=list(corrPars=list("1"=rep(log(0.1),8))), # 'init' optional
 lower=list(corrPars=list("1"=rep(log(1e-6),8))), # 'lower' and 'upper' required
 upper=list(corrPars=list("1"=rep(log(1e6),8)))))
exp(get_ranPars(by_cF)$corrPars[[1]]) # fitted variances
}
```

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### **Description**

This was the first function for fitting all spatial models in spaMM, and is still fully functional, but it is recommended to use fitme which has different defaults and generally selects more efficient fitting methods, and will handle all classes of models that spaMM can fit, including non-spatial ones. corrHLfit performs the joint estimation of correlation parameters, fixed effect and dispersion parameters.

### Usage

```
corrHLfit(formula, data, init.corrHLfit = list(), init.HLfit = list(),
    ranFix, fixed=list(), lower = list(), upper = list(),
    objective = NULL, resid.model = ~1,
    control.dist = list(), control.corrHLfit = list(),
    processed = NULL, family = gaussian(), method="REML",
    nb_cores = NULL, weights.form = NULL, ...)
```

### **Arguments**

formula Either a linear model formula (as handled by various fitting functions) or a

predictor, i.e. a formula with attributes (see Predictor and examples below).

See Details in spaMM for allowed terms in the formula.

data A data frame containing the variables in the response and the model formula.

init.corrHLfit An optional list of initial values for correlation and/or dispersion parameters,

e.g. list(rho=1,nu=1,lambda=1,phi=1) where rho and nu are parameters of the Matérn family (see Matern), and lambda and phi are dispersion parameters (see Details in spaMM for the meaning of these parameters). All are optional, but giving values for a dispersion parameter changes the ways it is estimated (see Details). rho may be a vector (see make\_scaled\_dist) and, in that case, it is possible that some or all of its elements are NA, for which corrHLfit substitutes

automatically determined values.

init. HLfit See identically named HLfit argument.

fixed, ranFix A list similar to init.corrHLfit, but specifying fixed values of the parameters

not estimated. ranFix is the old argument, maintained for back compatibility; fixed is the new argument, uniform across **spaMM** fitting functions. See

ranFix for further information.

lower An optional (sub)list of values of the parameters specified through init.corrHLfit,

in the same format as init.corrHLfit, used as lower values in calls to optim.

See Details for default values.

upper Same as lower, but for upper values.

objective For development purpose, not documented (this had a distinct use in the first

version of spaMM, but has been deprecated as such).

resid.model See identically named HLfit argument.

control.dist See control.dist in HLCor

control.corrHLfit

This may be used control the optimizer. See spaMM.options

for default values.

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processed For programming purposes, not documented.

family Either a family or a multi value.

method Character: the fitting method to be used, such as "ML", "REML" or "PQL/L".

"REML" is the default. Other possible values of HLfit's method argument are

handled.

weights.form Specification of prior weights by a one-sided formula: use weights.form = ~

pw instead of prior.weights = pw. The effect will be the same except that such an argument, known to evaluate to an object of class "formula", is suitable to

enforce safe programming practices (see good-practice).

nb\_cores Not yet operative, only for development purposes. Number of cores to use for

parallel computations.

... Optional arguments passed to HLCor, HLfit or mat\_sqrt, for example the distMatrix

argument of HLCor, or the verbose argument of HLfit. Arguments that do not fit within these functions are detected and a warning is issued. In a corrHLfit call, the verbose vector of booleans may include a TRACE=TRUE element, in which case information is displayed for each set of correlation and dispersion parameter values considered by the optimiser (see verbose for further informa-

tion, mostly useless except for development purposes).

#### **Details**

For approximations of likelihood, see method. For the possible structures of random effects, see random-effects,

By default corrHLfit will estimate correlation parameters by maximizing the objective value returned by HLCor calls wherein the dispersion parameters are estimated jointly with fixed effects for given correlation parameters. If dispersion parameters are specified in init.corrHLfit, they will also be estimated by maximizing the objective value, and HLCor calls will not estimate them jointly with fixed effects. This means that in general the fixed effect estimates may vary depending on init.corrHLfit when any form of REML correction is applied.

Correctly using corrHLfit for likelihood ratio tests of fixed effects may then be tricky. It is safe to perform full ML fits of all parameters (using method="ML") for such tests (see Examples). The higher level function fixedLRT is a safe interface for likelihood ratio tests using some form of REML estimation in corrHLfit.

attr(<fitted object>, "optimInfo")\$lower and ...\$upper gives the lower and upper bounds for optimization of correlation parameters. These are the default values if the user did not provide explicit values. For the adjacency model, the default values are the inverse of the maximum and minimum eigenvalues of the adjMatrix. For the Matérn model, the default values are not so easily summarized: they are intended to cover the range of values for which there is statistical information to distinguish among them.

### Value

The return value of an HLCor call, with additional attributes. The HLCor call is evaluated at the estimated correlation parameter values. These values are included in the return object as its \$corrPars member. The attributes added by corrHLfit include the original call of the function (which can be retrived by getCall(<fitted object>), and information about the optimization call within corrHLfit.

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#### See Also

See more examples on data set Loaloa, to compare fit times by corrHLfit and fitme. See fixedLRT for likelihood ratio tests.

### **Examples**

corrMatrix

Using a corrMatrix argument

#### Description

corrMatrix is an argument of HLCor, of class dist or matrix, with can be used if the model formula contains a term of the form corrMatrix(1|<...>). It describes a correlation matrix, possibly as a dist object. A covariance matrix can actually be passed through this argument, but then it must be a full matrix, not a dist object. The way the rows and columns of the matrix are matched to the rows of the data depends on the nature of the grouping term <...>.

The covStruct argument can be used for the same purpose and is much more general, in particular allowing to specify several correlation matrices.

#### **Details**

The simplest case is illustrated in the first two examples below: the grouping term is identical to a single variable which is present in the data, whose levels match the rownames of the corrMatrix. As illustrated by the second example, the order of the data does not matter in that case, because the factor levels are used to match the data rows to the appropriate row and columns of the corrMatrix. The corrMatrix may even contain rows (and columns) in excess of the levels of the grouping term, in which case these rows are ignored.

These convenient properties no longer hold when the grouping term is not a single variable from the data (third example below), or when its levels do not correspond to row names of the matrix.

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In these cases, (1) no attempt is made to match the data rows to the row and column names of the corrMatrix. Such attempt could succeed only if the user had given names to the matrix matching those that the called function could create from the information in the data, in which case the user should find easier to specify a single variable that can be matched; (2) the order of data and corrMatrix matter; Internally, a single factor variable is constructed from all levels of the variables in the grouping term (i.e., from all levels of latitude and longitude, in the third example), with levels 1,2,3... that are matched to rows 1,2,3... of the corrMatrix. Thus the first row of the data is always associated to the first row of the matrix; (3) further, the dimension of the matrix must match the number of levels implied by the grouping term. For example, one might consider the case of 14 response values but of correlations between only 7 levels of a random effect, with two responses for each level. Then the matrix must be of dimension 7x7.

```
data("blackcap")
## Here we manually reconstruct the correlation matrix
## of the ML fit produced by corrHLfit:
MLcorMat <- MaternCorr(proxy::dist(blackcap[,c("longitude","latitude")]),</pre>
                         nu=0.6285603, rho=0.0544659)
blackcap$name <- as.factor(rownames(blackcap))</pre>
## (1) Single variable present in the data
HLCor(migStatus ~ means+ corrMatrix(1|name), data=blackcap,
      corrMatrix=MLcorMat, method="ML")
## (2) Same, permuted: still gives correct result
perm <- sample(14)</pre>
# Permuted matrix (with permuted names) as 'dist' object
pmat <- as.matrix(MLcorMat)[perm,perm]</pre>
HLCor(migStatus ~ means+ corrMatrix(1|name),data=blackcap,
      corrMatrix=as.dist(pmat),method="ML")
#
# Permuted matrix (with permuted names) as correlation matrix
pcorr <- proxy::as.matrix(MLcorMat, diag=1)[perm,perm]</pre>
HLCor(migStatus ~ means+ corrMatrix(1|name),data=blackcap,
      corrMatrix=pcorr,method="ML")
## (3) Other grouping terms (note the messages):
HLCor(migStatus ~ means+ corrMatrix(1|longitude+latitude),data=blackcap,
      corrMatrix=MLcorMat, method="ML")
```

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### **Description**

corr\_family objects provide a convenient way to implement correlation models handled by spaMM, analogous to family objects. These objects are undocumented (but there are documentation pages for each of the models implemented).

### Usage

```
# Matern(...) # see help(Matern)
# Cauchy(...) # see help(Cauchy)
# corrMatrix(...) # see help(corrMatrix)
# AR1(...) # see help(AR1)
# adjacency(...) # see help(adjacency)
# IMRF(...) # see help(IMRF)
## S3 method for class 'corr_family'
print(x,...)
```

## **Arguments**

```
x corr_family object.
... arguments that may be needed by some corr_family object or some print method.
```

covStruct

Specifying correlation structures

### Description

covStruct is a formal argument of HLCor, also handled by fitme and corrHLfit, that allows one to specify the correlation structure for different types of random effects, It is an alternative to other ad hoc formal arguments such as corrMatrix or adjMatrix. It replaces the deprecated function Predictor(...) which has served as an interface for specifying the design matrices for random effects in early versions of spaMM.

The main use of covStruct is to specify the correlation matrix of levels of a given random effect term, or its inverse (a precision matrix). Assuming that the design matrix of each random effect term follows the structure **ZAL** described in random-effects, it is thus an indirect way of specifying the "square root" **L** of the correlation matrix. The optional **A** factor can also be given by the optional "AMatrices" attribute of covStruct.

covStruct is a list of matrices with names specifying the type of matrix considered:
covStruct=list(corrMatrix=<some matrix>) or covStruct=list(adjMatrix=<some matrix>),
where the "corrMatrix" or "adjMatrix" labels are used to specify the type of information provided
(accordingly, the names can be repeated: covStruct=list(corrMatrix=<.>,corrMatrix=<.>)).
NULL list members may be necessary, e.g.
covStruct=list(corrMatrix=<.>,"2"=NULL,corrMatrix=<.>))

```
covoci det-113t(corridati 1x-1.7)
```

when correlations matrices are required only for the first and third random effect.

The covariance structure of a corrMatrix(1|<grouping factor>) formula term can be specified in two ways (see Examples): either by a correlation matrix factor (covStruct=list(corrMatrix=<some

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matrix>)), or by a precision matrix factor  $\mathbf{Q}$  such that the covariance factor is  $\lambda \mathbf{Q}^{-1}$ , using the type name "precision": covStruct=list(precision=<some matrix>). The function as\_precision can be used to perform the conversion from correlation information to precision factor (using a crude solve() that may not always be efficient), but fitting functions may also perform such conversions automatically.

"AMatrices" is a list of matrices. The names of elements of the list does not matter, but the *i*th A matrix, and its row names, should match the *i*th **Z** matrix, and its column names. This implies that NULL list members may be necessary, as for the covStruct list.

# Usage

```
as_precision(corrMatrix, condnum=1e12)
```

# **Arguments**

corrMatrix Correlation matrix, specified as matrix or as dist object

condnum Numeric: when a standard Cholesky factorization fails, the matrix is regularized

so that the regularized matrix has this condition number (in version 3.10.0 this correction has been implemented more exactly than in previous versions).

### **Details**

```
covStruct can also be specified as a list with an optional "types" attribute, e.g. structure(list(<some matrix>, types="corrMatrix")).
```

### Value

as\_precision returns a list with additional class precision and with single element a symmetric matrix of class dsCMatrix.

### See Also

Gryphon and pedigree for a type of applications where declaring a precision matrix is useful.

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diallel

Random-effect structures for diallel experiments and other dyadic interactions

### **Description**

ranGCA and diallel are random-effect structures designed to represent the effet of symmetric interactions between pairs of individuals (order of individuals in the pair does not matter), while antisym represents anti-symmetric interactions (the effect of reciprocal ordered pairs on the outcome are opposite, as in the so-called Bradley-Terry models). These random-effect structures all account for multiple membership, i.e., the fact that the same individual may act as the first or the second individual among different pairs, or even within one pair if this makes sense).

More formally, the outcome of an interaction between a pair i,j of agents is subject to a symmetric overall random effect  $v_{ij}$  when the effect "on" individual i (or viewed from the perspective of individual i) equals the effect on j:  $v_{ij} = v_{ji}$ . This may result from the additive effect of individual random effects  $v_i$  and  $v_j$ :  $v_{ij} = v_i + v_j$ , but also from non-additive effects  $v_{ij} = v_i + v_j + a_{ij}$  if the interaction term  $a_{ij}$  is itself symmetric ( $a_{ij} = a_{ji}$ ). ranGCA and diallel effects represent such symmetric effects, additive or non-additive respectively, in a model formula (see Details for the semantic origin of these names and how they can be changed). Conversely, antisymmetry is characterized by  $v_{ij} = v_i - v_j = -v_{ji}$  and is represented by the antisym formula term.

If individual-level random effects of the form (1IID1)+ (1IID2) were included in the model formula instead of ranGCA(1|ID1+ID2) for symmetric additive interactions, this would result in different variances being fitted for each random effect (breaking the assumption of symmetry), and the value of the random effect would differ for an individual whether it appears as a level of the first random effect or of the second (which is also inconsistent with the idea that the random effect represents a property of the individual).

When ranGCA or antisym random effects are fitted, the individual effects are inferred. By contrast, when a diallel random effect is fitted, an autocorrelated random effect  $v_{ij}$  is inferred for each **unordered** pair (no individual effect is inferred), with correlation  $\rho$  between levels for pairs sharing one individual. This correlation parameter is fitted and is constrained by  $\rho < 0.5$  (see Details). ranGCA is equivalent to the case  $\rho = 0.5$ . diallel fits can be slow for large data if the correlation matrix is large, as this matrix can have a fair proportion of nonzero elements. There may also be identifiability issues for variance parameters: in a LMM as shown in the examples, there will be three parameters for the random variation (phi, lambda and rho) but only two can be estimated if only one observation is made for each dyad.

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### Usage

```
## formula terms:

# ranGCA(1| <.> + <.>)
# antisym(1| <.> + <.>)
# diallel(1| <.> + <.>, tpar, fixed = NULL, public = NULL)

## where the <.> are two factor identifiers, ** whose levels
## must be identical when representing the same individual **

## corrFamily constructors:
ranGCA() # no argument
antisym() # no argument
diallel(tpar, fixed = NULL, public = NULL)
```

### **Arguments**

tpar Numeric: template value of the correlation coefficient for pairs sharing one in-

dividual.

fixed NULL or fixed value of the correlation coefficient.

public NULL, or an environment. When an empty environment is provided, a template

CorNA for the correlation matrix (with NA's in place of  $\rho$ ) will be copied therein,

for inspection at user level.

### **Details**

Although the symmetric random-effect structures may be used in many different contexts (including social network analysis, or "round robin" experiments in psychology; another possibly relevant literature keyword here is "multi membership"), their present names refer to the semantics established for diallel experiments (e.g., Lynch & Walsh, 1998, p. 611), because it is not easy to find a more general yet intuitive semantics. If the names ranGCA and diallel sound inappropriate for your context of application, you can declare and use an alternative name for them, taking advantage of the fact that they are random-effect structures defined through corrFamily constructors, which are functions named as the formula term. For example, symAdd(1|ID1+ID2) can be used in a model formula after the following two steps:

```
# Define the 'symAdd' corrFamily constructor (a function) by copy:
symAdd <- ranGCA
# Associate the 'symAdd' function to 'symAdd' formula terms:
register_cF("symAdd")</pre>
```

In diallel experiments, one analyzes the phenotypes of offspring from multiple crosses among which the mother in a cross can be the father in another, so this is an example of multiple-membership. The additive genetic effects of each parent's genotypes are described as "general combining abilities" (GCA). In case of non-additive effect, the half-sib covariance is not half the full-sib covariance and this is represented by the interaction  $a_{ij}$  described as "specific combining abilities" (SCA). The sum of GCA and SCA defines a synthetic random effect "received" by the offspring, with distinct levels

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for each unordered parental pair, and with correlation  $\rho$  between effects received by half-sibs (one shared parent).  $\rho$  corresponds to var(GCA)/[2\*var(GCA)+var(SCA)] and is necessarily  $\leq 0.5$ .

See the X. GCA documentation for similar constructs for fixed effects.

### Value

The functions return corrFamily descriptors whose general format is described in corrFamily. The ones produced by ranGCA and antisym are atypical in that only their Af element is non-trivial.

#### References

Lynch, M., Walsh, B. (1998) Genetics and analysis of quantitative traits. Sinauer, Sunderland, Mass.

```
#### Simulate dyadic data
set.seed(123)
nind <- 10
                  # Beware data grow as O(nind^2)
x <- runif(nind^2)</pre>
id12 <- expand.grid(id1=seg(nind),id2=seg(nind))</pre>
id1 <- id12$id1
id2 <- id12$id2
u \leftarrow rnorm(nind, mean = 0, sd=0.5)
## additive individual effects:
y \leftarrow 0.1 + 1*x + u[id1] + u[id2] + rnorm(nind^2, sd=0.2)
## Same with non-additive individual effects:
dist.u \leftarrow abs(u[id1] - u[id2])
z <- 0.1 + 1*x + dist.u + rnorm(nind^2, sd=0.2)
## anti-smmetric individual effects:
t < 0.1 + 1*x + u[id1] - u[id2] + rnorm(nind^2, sd=0.2)
dyaddf <- data.frame(x=x, y=y, z=z, t=t, id1=id1,id2=id2)</pre>
# : note that this contains two rows per dyad, which avoids identifiability issues.
# Enforce that interactions are between distinct individuals (not essential for the fit):
dyaddf <- dyaddf[- seg.int(1L,nind^2,nind+1L),]</pre>
# Fits:
(addfit <- fitme(y ~x +ranGCA(1|id1+id2), data=dyaddf))</pre>
# practically equivalent to:
(fitme(y ~x +diallel(1|id1+id2, fixed=0.49999), data=dyaddf))
(antifit <- fitme(t ~x +antisym(1|id1+id2), data=dyaddf))</pre>
```

54 div\_info

```
(distfit <- fitme(z ~x +diallel(1|id1+id2), data=dyaddf))</pre>
```

div\_info

Information about numerical problems

# Description

This experimental function displays information about parameter values for which some numerical problems have occurred. Some warnings suggest its use.

Numerical problems may occur if the information matrix (for the augmented linear model used in the iteratively reweighted least-squares algorithm) is nearly singular. **spaMM** may try to check whether such singularity occurs when this algorithm has not converged. But itself may be slow so it is not performed systematically for large matrices. spaMM.options(diagnose\_conv=<integer>) may be used to control the maximum size of matrices for which the check is performed.

When "outer" generic optimization is performed, information is reported about the range of parameter values for which problems occurred, (see Value). The fit object divinfo element may also contain more informative tables of parameter values. This information is currently missing for "inner"-optimized parameters.

### Usage

```
div_info(object, ...)
```

# **Arguments**

object An object of class HLfit, as returned by the fitting functions in spaMM.

Currently not used

# Value

Used mainly for the side effects (printed output) but returns invisibly either a single parameter vector (if a single numerical problem occurred) or a matrix of parameter ranges, or NULL if there is no problem to report.

```
# Tragically ;-), no simple example of numerical problems
# that can be diagnosed by div_info() is currently available.
```

DoF

Degrees of freedom extractor

### **Description**

This extracts the number of degrees of freedom for a model, in the usual sense for likelihood-ratio tests: a count of number of fitted parameters, distinguishing different classes of parameters (see Value).

## Usage

DoF(object)

# **Arguments**

object

A fitted-model object, of class "HLfit".

#### **Details**

The output distinguishes counts of random-effect vs residual-dispersion parameters, following the conceptual distinction between effects that induce correlations between different levels of the resonse vs. observation-level effects. However, a residual-dispersion component can be declared as a random effect, so that the counts for logically equivalent models may differ according to the way a model was declared. For example if residual dispersion for an LLM is declared as an observation-level random effect while phi is fixed, the p\_lambda component will include 1 df for what would otherwise be accounted by the p\_rdisp component. A more involved case where the same contrast happens is when a negative-binomial model (with a residual-dispersion shape parameter) is declared as a Poisson-gamma mixture model (with a varaince parameter for the Gamma-distributed individual-level random effect).

### Value

A vector with possible elements p\_fixef, p\_lambda, p\_corrPars and p\_rdisp for, respectively, the number of fixed-effect coefficients of the main-response model, the number of random-effect variance parameters, the number of random-effect correlation parameters, and the number of residual dispersion parameters (the latter being itself, for a mixed-effect residual-dispersion model, the sum of such components).

### See Also

df.residual.HLfit; get\_any\_IC for extracting effective degrees of freedom considered in the model-selection literature; as\_LMLT for access to the effective degrees of freedom considered in Satterthwaite's test and its extentions.

56 dofuture

dofuture Interface for parallel computations	
dofuture Interface for parallel computations	

# Description

interface to apply some function fn in parallel on columns of a matrix. It is not logically restricted to mixed-effect applications, hence it can be used more widely. Depending on the nb\_cores argument, parallel or serial computation is performed, calling the future.apply::future\_apply function. A socket cluster is used by default for parallel computations, but a fork cluster can be requested on linux and alike operating systems by using argument cluster\_args=list(type="FORK").

# Usage

```
dofuture(newresp, fn, nb_cores=NULL, fit_env, control=list(),
      cluster_args=NULL, debug.=FALSE, iseed=NULL,
      showpbar="ignored", pretest_cores="ignored",
      ...)
```

sibly to fn).

# **Arguments**

	newresp	A matrix on whose columns fn will be applied (e.g., as used internally in <b>spaMM</b> , the return value of a simulate.HLfit() call); or an integer, then converted to a trivial matrix (seq(newresp), ncol=newresp, nrow=1).
	fn	Function whose first argument is named y. The function will be applied for y taken to be each column of newresp.
	nb_cores	Integer. Number of cores to use for parallel computations. If >1, a cluster of nb_cores nodes is used. Otherwise, no parallel computation is performed.
	fit_env	(for socket clusters only:) An environment, or a list, containing variables to be exported on the nodes of the cluster (by parallel::clusterExport).
	control	A list. The only effective control is .combine="rbind" (mimicking the foreach syntax used in the alternative interface dopar).
	cluster_args	A list of arguments passed to parallel::makeCluster or parallel::makeForkCluster. E.g., outfile="log.txt" may be useful to collect output from the nodes, and type="FORK" to force a fork cluster on linux(-alikes).
	debug.	(for socket clusters only:) For debugging purposes. Effect, if any, is to be defined by the fn as provided by the user.
	iseed	Integer, or NULL. If an integer, it is used to initialize "L'Ecuyer-CMRG" random- number generator (iseed argument of clusterSetRNGStream), with identical effect across different models of parallelisation. If iseed is NULL, the seed is not controlled.
showpbar, pretest_cores		
		Currently ignored; for consistency with dopar formal arguments.
	• • •	Further arguments to be passed (unevaluated) to future.apply (and then pos-

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#### Value

The result of calling future.apply. If the progressr package is loaded, a side-effect of dofuture is to show a progress bar with character 'S' or 'P' or 'F' depending on parallelisation status (serial/socket/fork).

#### See Also

dopar for an alternative implementation of (essentially) the same functionalities, and wrap\_parallel for its differences from dofuture.

### **Examples**

```
## Not run:
if (requireNamespace("future.apply", quietly = TRUE)) {

# Useless function, but requiring some argument beyond the first
foo <- function(y, somearg, ...) {
   if ( is.null(somearg) || TRUE ) length(y)
}

# Whether FORK can be used depends on OS and whether Rstudio is used:
   dofuture(matrix(1,ncol=4,nrow=3), foo, fit_env=list(), somearg=NULL,
        nb_cores=2, cluster_args=list(type="FORK"))
}

## End(Not run)</pre>
```

dopar

Interface for parallel computations

### Description

dopar and combinepar are interfaces primarily designed to apply some function fn in parallel on columns of a matrix, although other uses are possible. Depending on the nb\_cores argument, parallel or serial computation is performed. A socket cluster is used by default for parallel computations, but a fork cluster can be requested on linux and alike operating systems by using argument cluster\_args=list(type="FORK").

dopar has been designed to provide by default a progress bar in all evaluations contexts. A draw-back is that different procedures are called depending e.g. on the type of cluster, with different possible controls. In particular, foreach is called in some cases but not others, so non-trivial values of its . combine control are not always enforced. The alternative interface combinepar will always use foreach, and will still try to provide by default a progress bar but may fail to do so in some cases (see Details).

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#### Usage

```
dopar(newresp, fn, nb_cores = NULL, fit_env,
   control = list(.final=function(v) if( ! is.list(v[[1]])) {do.call(cbind,v)} else v),
     cluster_args = NULL, debug. = FALSE, iseed = NULL,
     showpbar = eval(spaMM.getOption("barstyle")),
     pretest_cores =NULL, ...)
combinepar(newresp, fn, nb_cores = NULL, cluster=NULL, fit_env,
   control = list(.final=function(v) if( ! is.list(v[[1]])) {do.call(cbind,v)} else v),
     cluster_args = NULL, debug. = FALSE, iseed = NULL,
     showpbar = eval(spaMM.getOption("barstyle")),
     pretest_cores =NULL, ...)
```

#### **Arguments**

A matrix on whose columns fn will be applied (e.g., as used internally in **spaMM**, newresp

the return value of a simulate. HLfit() call); or an integer, then converted to a

trivial matrix matrix(seq(newresp), ncol=newresp, nrow=1).

fn Function whose first argument is named y. The function will be applied for y

taken to be each column of newresp.

nb\_cores Integer. Number of cores to use for parallel computations. If >1 (and no cluster

is provided by the cluster argument), a cluster of nb\_cores nodes is created, used, and stopped on completion of the computation. Otherwise, no parallel

computation is performed.

cluster (for combinepar only): a cluster object (as returned by parallel::makeCluster

> or parallel::makeForkCluster). If this is used, the nb\_cores and cluster\_args arguments are ignored. The cluster is not stopped on completion of the compu-

tation

fit\_env (for socket clusters only:) An environment, or a list, containing variables to

be exported on the nodes of the cluster (by parallel::clusterExport); e.g.,

list(bar=bar) to pass object bar to each node. The argument control(.errorhandling

= "pass"), below, is useful to find out missing variables.

A list following the foreach control syntax, even if foreach is not used. There are limitations when dopar (but not combinepar) is used, in all but the first case below:

> 1. for socket clusters, with doSNOW attached, for each is called with default arguments including i = 1:ncol(newresp), .inorder = TRUE, .errorhandling = "remove", .packages = "spaMM", and further arguments taken from the present function's control argument, which may also be used to override the defaults. For example, .errorhandling = "pass" is useful to get error messages from the nodes, and therefore strongly recommended when first experimenting with this function.

2. for socket clusters, with doSNOW **not** attached, dopar calls phapply instead of foreach but control\$.packages is still handled. The result is still in the format returned in the first case, i.e. by foreach, taking the control argument into account. pbapply arguments may be passed through the ... argument.

control

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3. if a fork cluster is used, dopar calls mclapply instead of foreach. control\$mc.silent can be used to control the mc.silent argument of mclapply.

4. (if nb\_cores=1 dopar calls mclapply).

cluster\_args A list of arguments passed to parallel::makeCluster. E.g., outfile="log.txt"

may be useful to collect output from the nodes, and type="FORK" to force a fork

cluster on linux(-alikes).

debug. (for socket clusters only:) For debugging purposes. Effect, if any, is to be defined

by the fn as provided by the user.

iseed (all parallel contexts:) Integer, or NULL. If an integer, it is used as the iseed

argument of clusterSetRNGStream to initialize "L'Ecuyer-CMRG" random-number generator (see Details). If iseed is NULL, the default generator is se-

lected on each node, where its seed is not controlled.

showpbar (for socket clusters only:) Controls display of progress bar. See barstyle option

for details.

pretest\_cores (for socket clusters only:) A function to run on the cores before running fn.

It may be used to check that all arguments of the fn can be evaluated in the cores' environments (the internal function .pretest\_fn\_on\_cores provides an

example).

.. Further arguments to be passed (unevaluated) to fn, if not caught on the way

by pbapply (which means that different results may in principle be obtained depending on the mode of parallelisation, which is the kind of design issues that

combinepar aims to resolve by always calling foreach).

#### **Details**

Control of random numbers through the "L'Ecuyer-CMRG" generator and the iseed argument is not sufficient for consistent results when the doSNOW parallel backend is used, so if you really need such control in a fn using random numbers, do not use doSNOW. Yet, it is fine to use doSNOW for bootstrap procedures in spaMM, because the fitting functions do not use random numbers: only sample simulation uses them, and it is not performed in parallel.

combinepar calls foreach:: %dopar% which assumes that a cluster has been declared using a suitable backend such as doSNOW, doFuture or doParallel. If only the latter is available, no progress bar is displayed. A method to render a bar when doParallel is used can be found on the Web, but that bar is not a valid progress bar as it is displayed only after all the processes have been run.

## Value

The result of calling foreach, pbapply or mclapply, as dependent on the control argument and the interface used. A side-effect of either interface is to show a progress bar whose character informs about the type of parallelisation performed: a "F" or default "=" character for fork clusters, a "P" for parallel computation via foreach and doSNOW, a "p" for parallel computation via foreach and doFuture or via pbapply, and "s" for serial computation foreach and doParallel or via pbapply.

#### See Also

dofuture is yet another interface with (essentially) the same functionalities as dopar. See the documentation of the wrap\_parallel option for its differences from dopar.

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### **Examples**

```
## See source code of spaMM_boot()
## Not run:
# Useless function, but requiring some argument beyond the first
foo <- function(y, somearg, ...) {
   if ( is.null(somearg) || TRUE ) length(y)
}

# Whether FORK can be used depends on OS and whether Rstudio is used:
dopar(matrix(1,ncol=4,nrow=3), foo, fit_env=list(), somearg=NULL,
   nb_cores=2, cluster_args=list(type="FORK"))

## End(Not run)</pre>
```

drop1.HLfit

Drop all possible single fixed-effect terms from a model

### **Description**

Drop single terms from the model. The drop1 method for **spaMM** fit objects is conceived to replicate the functionality, output format and details of pre-existing methods for similar models. Results for LMs and GLMs should replicate base R drop1 results, with some exceptions:

- \* somewhat stricter default check of non-default scope argument;
- \* Because the dispersion estimates for Gamma GLMs differ between stats::glm and **spaMM** fits (see Details in method), some tests may differ too; results from **spaMM** REML fits being closer than ML fits to those from glm() fits;
- \* AIC values reported in tables are always the marginal AIC as computed by AIC.HLfit, while drop1.glm may report confusing (to me, at least) values (see AIC.HLfit) for reasons that seem to go beyond differences in dispersion estimates.

For LMMs, ANOVA tables are provided by interfacing lmerTest::anova (with non-default type).

For other classes of models, a table of likelihood ratio tests is returned, each test resulting from a call to LRT.

# Usage

```
## S3 method for class 'HLfit'
drop1(object, scope, method="", check_marg=NULL, check_time=60, ...)
```

#### **Arguments**

object Fit object returned by a **spaMM** fitting function.

scope Default "scope" (terms to be tested, specified as a formula, see Examples) is

determined by applying stats::drop.scope on fixed-effect terms. Non-default scope can be specified a formula giving the terms to be considered for dropping. It is also possible to specify them as a character vector, but then one has to make

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sure that the elements are consistent with term labels produced by terms, as inconsistent elements will be ignored.

method Only non-default value is "LRT" which forces evaluation of a likelihood ratio

tests by LRT, instead of specific methods for specific classes of models.

check\_marg NULL or boolean: whether effects should be checked for marginality. By de-

fault, this check is performed when a non-default scope is specified, and then no test is reported for terms that do not satisfy the marginality condition. If check\_marg=FALSE, marginality is not checked and tests are always performed.

check\_time numeric: whether to output some information when the execution time of drop1

may be of the order of the time specified by check\_time, or more. This is checked only when random effect are present. Such output can thus be sup-

pressed by check\_time=Inf.

... Further arguments passed from or to methods, or to LRT.

#### **Details**

As for the ANOVA-table functionality, it has been included here mainly to provide access to F tests (including, for LMMs, the "Satterthwaite method", using pre-existing procedures as template or backend for expediency and familiarity. The procedures for specific classes of models have various limitations, e.g., none of them handle models with variable dispersion parameter. For classes of models not well handled by these procedures (by design or due to the experimental nature of the recent implementation), method="LRT" can still be applied (and will be applied by default for GLMMs).

# Value

The return format is that of the function called (lmerTest::drop1 for LMMs), or emulated (base drop1 methods for LMs or GLMs), or is a data frame whose rows are each the result of calling LRT.

# See Also

```
as_LMLT for the interface to lmerTest::drop1.
```

62 eval\_replicate

eval\_replicate

Evaluating bootstrap replicates

# **Description**

eval\_replicate is the default simuland function applied to simulated bootstrap samples by likelihoodratio testing functions (fixedLRT, LRT, anove.HLfit). This documentation presents the requirements and possible features of this function and of possible user-defined alternatives.

An alternative function spaMM:::.eval\_replicate2 is also provided. It is slower, as it refits the models compared with different initial values for random-effect parameters, which is useful in some difficult cases where initial values matter. The eval\_replicate function may also refit the "full" models with different initial values when the logLik of the refitted full model is substantially lower than that of the refitted null model. "Substantially" means that a tolerance of 1e-04 is applied to account for inaccuracies of numerical maximization.

### Usage

```
eval_replicate(y)
```

#### **Arguments**

У

a response vector on which a previously fitted model may be refitted.

### Details

likelihood-ratio testing functions have a debug. argument whose effect depends on the simuland function. The default behaviour is thus defined by eval\_replicate, as: if debug.=TRUE, upon error in the fitting procedures, dump.frames will be called, in which case **a dump file will be written on disk**; and a **list** with debugging information will be returned (so that, say, pbapply will not return a matrix). This behaviour may change in later versions, so non-default debug. values should not be used in reproducible code. In serial computation, debug.=2 may induce a stop; this should not happen in parallel computation because the calling functions check against debug.==2.

Essential information such as the originally fitted models is passed to the function not as arguments but through its environment, which is controlled by the calling functions (see the eval\_replicate source code to know which are these arguments). Users should thus not assume that they can control their own simuland function's environment as this environment will be altered.

Advanced users can define their own simuland function. The eval\_replicate source code provides a template showing how to use the function's environment. The Example below illustrates another approach augmenting eval\_replicate. A further example is provided in the file tests/testthat/test-LRT-boot.R, using ... to pass additional arguments beyond response values.

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#### Value

A vector of the form c(full=logLik(<refitted full model>), null=logLik(<refitted null model>); or possibly in debugging contexts, a list with the same elements each with some additional information provided as attribute.

#### See Also

Calling functions fixedLRT, LRT.

### **Examples**

```
## Not run:
# Simple wrapper enhancing the default 'simuland'
# with a call to some obscure option, and dealing with
# the need to pass the environment assigned to 'simuland'
eval_with_opt <- function(y) {
    spaMM.options(some_obscure_option="some_obscure_value")
    eval_rep <- spaMM:::.eval_replicate
    environment(eval_rep) <- parent.env(environment()) # passing the environment
    eval_rep(y)
}
## End(Not run)</pre>
```

external-libraries

Installing external libraries

# Description

spaMM is conceived to minimize installation issues but it nevertheless suggests using some external libraries. These are all accessed through R packages so their installation should be easy when installing binary packages. The Details below give hints for installing packages from source. They may all be obsolete if you are using the Rtools42 on Windows. For all cases not considered below, help yourself. If you are using the Rtools40 on Windows, you should have a look at the package manager in the Rtools40 bash shell.

### **Details**

The ROI.plugin.glpk package requires the Rglpk package, which itself requires the external glpk library. For the latter, Debian-ists and alikes should sudo apt-get install libglpk-dev. MacOSX users should brew install glpk if using brew; Windows users should try using pacman -S mingw-w64-x86\_64-glpk in the Rtools40 bash shell, together with Sys.setenv(GLPK\_HOME = "\$(MINGW\_PREFIX)") in the R session (but I have not fully tested this; previously I had to install glpk from https://sourceforge.net/projects/winglpk/).

The nloptr package requires the external NLopt library. Windows users should try using pacman -S mingw-w64-x86\_64-nlopt in the Rtools40 bash shell (but again I have not fully tested this; see also the README of nloptr). To install nloptr 2.0.0 from sources on Debian one may have to install libnlopt-dev: sudo apt-get install libnlopt-dev Likewise for gmp one may need to install libgmp3-dev.

64 extractors

extractors

Functions to extract various components of a fit.

# **Description**

Most extractors are methods of generic functions defined in base R (see Usage), for which the base documentation may be useful.

formula extracts the model formula.

family extracts the response family.

terms extracts the formula, with attributes describing the **fixed-effect** terms.

nobs returns the length of the response vector.

logLik extracts the log-likelihood (exact or approximated).

dev\_resids returns a vector of squared (unscaled) deviance residuals (the summands defined for GLMs in McCullagh and Nelder 1989, p. 34; see Details of LL-family for other response families. deviance returns the sum of squares of these deviance residuals, possibly weighted by prior weights (consistently with stats::deviance. See residuals.HLfit for details and comparison with related extractors.

fitted extracts fitted values.

response extracts the response (as a vector).

fixef extracts the fixed effects coefficients,  $\beta$ .

ranef extracts the predicted random effects, **Lv** (default since version 1.12.0), or optionally **u** (see random-effects for definitions). print.ranef controls their printing.

getDistMat returns a distance matrix for a geostatistical (Matérn etc.) random effect.

df.residual extracts residual degrees-of-freedom for fitted models (here number of observations minus number of parameters of the model except residual dispersion parameters). wweights extracts prior weights (as defined by the fitting functions's prior.weights argument).

# Usage

```
## S3 method for class 'HLfit'
formula(x, which="hyper", ...)
## S3 method for class 'HLfit'
family(object, ...)
## S3 method for class 'HLfit'
terms(x, ...)
## S3 method for class 'HLfit'
nobs(object, ...)
## S3 method for class 'HLfit'
logLik(object, which, ...)
## S3 method for class 'HLfit'
fitted(object, ...)
## S3 method for class 'HLfit'
fixef(object, na.rm=NULL, ...)
## S3 method for class 'HLfit'
ranef(object, type = "correlated", ...)
## S3 method for class 'ranef'
```

65 extractors

```
print(x, max.print = 40L, ...)
## S3 method for class 'HLfit'
deviance(object, ...)
## S3 method for class 'HLfit'
df.residual(object, ...)
## S3 method for class 'HLfit'
weights(object, type, ...)
getDistMat(object, scaled=FALSE, which = 1L)
response(object,...)
dev_resids(object,...)
```

#### **Arguments**

object An object of class HLfit, as returned by the fitting functions in spaMM.

For ranef, use type="correlated" (default) to display the correlated rantype dom effects (Lv), whether in a spatial model, or a random- coefficient model. Use type="uncorrelated" to pretty-print the elements of the <object>\$ranef

vector (u).

For weights, either "prior" or "working", with the same meaning as for weights.glm: respectively the prior weights, or the weights used in the final

iteration of the IRLS algorithm.

\* For logLik, the name of the element of the APHLs list to return (see Details for any further possibility). The default depends on the fitting method. In particular, if it was REML or one of its variants, the default is to return the log restricted likelihood (exact or approximated).

\* For getDistMat, an integer, to select a random effect from several for which a distance matrix may be constructed.

\* For formula, by default the model formula with non-expanded multIMRF random-effect terms is returned, while for which="" a formula with multIMRF terms expanded as IMRF terms is returned.

Whether to include NA values for missing coefficients of rank-deficient model matrices. Default is to exclude them for mixed models and to include them for

other ones. See Details for the underlying reason.

If FALSE, the function ignores the scale parameter  $\rho$  and returns unscaled disscaled

tance

For print.ranef: the return value of ranef.HLfit. Х

Controls options("max.print") locally. max.print

Other arguments that may be needed by some method.

#### **Details**

For rank-deficient model matrices, base R procedures 1m and g1m estimate coefficients for a ranktrimmed matrix and coefficient() returns a full-length vector completed with NA values for coefficients not estimated, while the lme4 fixef method returns a trimmed vector. spaMM has long followed the base R convention for all models but this may impede use of some post-fit procedures initially conceived for lme4 objects (such as lmerTest procedures for LMMs). So now

which

na.rm

66 extreme\_eig

fixef.HLfit trims the vector by default for mixed-effect models only. The default is thus to maximize consistency/compatibility with preexisting procedures despite their inconsistencies with each other.

# Value

formula returns a formula, except a list of them from fitmv() output.

terms returns an object of class c("terms", "formula") which contains the *terms* representation of a symbolic model. See terms.object for its structure. terms(<fitmv() result>) returns a list of such terms.

Other return values are numeric (for logLik), vectors (most cases), matrices or dist objects (for getDistMat), or a family object (for family). ranef returns a list of vectors or matrices (the latter for random-coefficient terms).

### References

McCullagh, P. and Nelder J. A. (1989) Generalized linear models. Second ed. Chapman & Hall: London.

#### See Also

See summary. HLfit whose return value include the tables of fixed-effects coefficients and random-effect variances displayed by the summary, residuals. HLfit to extract various residuals, residVar to extract residual variances or information about residual variance models, hatvalues to extract leverages, get\_matrix to extract the model matrix and derived matrices, and vcov.HLfit to extract covariances matrices from a fit, get\_RLRsim\_args to extract arguments for (notably) tests of random effects in LMMs.

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## **Description**

regularize can be used to regularize (nearly-)singular correlation matrices. It may also be used to regularize covariance matrices but will not keep their diagonal constant. Use on other types of matrices may give nonsense. The regularization corrects the diagonal of matrices with high condition number so that the condition number of a corrected matrix is the maximum value specified by maxcondnum. For that purpose, it needs the extreme eigenvalues of the matrix, by default provided by the function extreme\_eig. Calls functions from **RSpectra** if available, and falls back on base functions otherwise.

# Usage

```
extreme_eig(M, symmetric, required = TRUE)
regularize(A, EEV=extreme_eig(A,symmetric=TRUE), maxcondnum=1e12)
```

# **Arguments**

М	Square matrix. Sparse matrices of class d[s g]CMatrix (and some others too) are handled (some vagueness, as if it fails for some matrix types, an alternative function should be easy to define based on this one as template.
Α	Square matrix as M, assumed symmetric.
symmetric	Whether the matrix is symmetric. Helpful to select efficient methods for this case if the matrix class does not implies its symmetry.
required	Whether the computation should be attempted independently of the size of the matrix.
EEV	Two extreme eigenvalue in the return format of extreme_eig
maxcondnum	Target condition number when regularization is performed

### Value

extreme\_eig returns a vector of length 2, the largest and the smallest eigenvalues in this order. regularize returns a matrix, possibly in sparse format.

```
H10 <- Matrix::Hilbert(10)
extreme_eig(H10,symmetric=TRUE) # ratio > 1e13
rH10 <- regularize(H10)
extreme_eig(rH10,symmetric=TRUE) # ratio = 1e12
```

68 fitme

fitme

Fitting function for fixed- and mixed-effect models with GLM response.

### **Description**

This is a common interface for fitting most models that spaMM can fit, from linear models to mixed models with non-gaussian random effects, therefore substituting to corrHLfit, HLCor and HLfit. By default, it uses ML rather than REML (differing in this respect from the other fitting functions). It may use "outer optimization", i.e., generic optimization methods for estimating all dispersion parameters, rather than the iterative methods implemented in HLfit. The results of REML fits of non-gaussian mixed models by these different methods may (generally slightly) differ. Outer optimization should generally be faster than the alternative algorithms for large data sets when the residual variance model is a single constant term (no structured dispersion). For mixed models, fitme by default tries to select the fastest method when both can be applied, but precise decision criteria are subject to change in the future. corrHLfit (with non-default arguments to control the optimization method most suitable to a particular problem) may be used to ensure better consistency over successive versions of spaMM.

### **Usage**

```
fitme(formula, data, family = gaussian(), init = list(), fixed = list(),
     lower = list(), upper = list(), resid.model = ~1, init.HLfit = list(),
     control = list(), control.dist = list(), method = "ML",
     HLmethod = method, processed = NULL, nb_cores = NULL, objective = NULL,
     weights.form = NULL, ...)
```

#### **Arguments**

init

formula

Either a linear model formula (as handled by various fitting functions) or a predictor, i.e. a formula with attributes (see Predictor and examples below). See Details in spaMM for allowed terms in the formula.

data A data frame containing the variables in the response and the model formula.

family Either a response family or a multi value.

> An optional list of initial values for correlation and/or dispersion parameters and/or response family parameters, e.g. list(rho=1, nu=1, lambda=1, phi=1)

where rho and nu are parameters of the Matérn family (see Matern), and lambda and phi are dispersion parameters (see Details in spaMM for the meaning of these parameters). All are optional, but giving values for a dispersion parameter changes the ways it is estimated (see Details and Examples). rho may be a vector (see make\_scaled\_dist) and, in that case, it is possible that some or all of its elements are NA, for which fitme substitutes automatically determined

values.

A list similar to init, but specifying fixed values of the parameters not estimated. See fixed for further information; and keep in mind that fixed fixedeffect coefficients can be passed as the etaFix argument as part of the '...'.

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lower An optional (sub)list of values of the parameters specified through init, in the

same format as init, used as lower values in calls to optim. See Details for

default values.

upper Same as lower, but for upper values.

resid.model See identically named HLfit argument.
init.HLfit See identically named HLfit argument.

control.dist See control.dist in HLCor

method, HLmethod

Character: the fitting method to be used, such as "ML", "REML" or "PQL/L". "ML" is the default, in contrast to "REML" for HLfit, HLCor and corrHLfit. Other possible values of HLfit's method argument are handled. method=c(<"ML" or "REML">, "exp") can be distinctly useful for slow fits of models with Gamma(log) response family (see method).

weights.form

Specification of prior weights by a one-sided formula: use weights.form = ~pw instead of prior.weights = pw. The effect will be the same except that such an argument, known to evaluate to an object of class "formula", is suitable to enforce safe programming practices (see good-practice).

control A list of (rare

A list of (rarely needed) control parameters, with possible elements:

- refit, a boolean, or a list of booleans with possible elements phi, lambda and ranCoefs. If either element is set to TRUE, then the corresponding parameters are refitted by the internal HLfit methods (see Details), unless these methods were already selected for such parameters in the main fitting step. If refit is a single boolean, it affects all parameters. By default no parameter is refitted.
- optimizer, the numerical optimizer, specified as a string and whose default is controlled by the global **spaMM** option "optimizer". Possible values are "nloptr", "bobyqa", "L-BFGS-B" and ".safe\_opt", whose meanings are detailed in the documentation for the optimizer argument of spaMM.options. Better left unchanged unless suspect fits are obtained.
- nloptr, itself a list of control parameters to be copied in the opts argument of nloptr. Default value is given by spaMM.getOption('nloptr') and possibly other global **spaMM** options. Better left unchanged unless you are ready to inspect source code.
- bobyqa, optim, lists of controls similar to nloptr but for methods "bobyqa" and "L-BFGS-B", respectively.

nb\_cores

For development purpose, not documented.

processed

For programming purpose, not documented.

objective

For development purpose, not documented.

Optional arguments passed to (or operating as if passed to) HLCor, HLfit or mat\_sqrt, for example rand. family, control. HLfit, verbose or the distMatrix argument of HLCor (so that estimation of Matern or Cauchy parameters can be combined with use of an ad hoc distance matrix). In a fitme call, the verbose vector of booleans may include a TRACE=TRUE element, in which case information is displayed for each set of correlation and dispersion parameter values considered by the optimiser (see verbose for further information, mostly useless except for development purposes).

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#### **Details**

For approximations of likelihood, see method. For the possible structures of random effects, see random-effects,

For phi, lambda, and ranCoefs, fitme may or may not use the internal fitting methods of HLfit. The latter methods are well suited for structured dispersion models, but require computations which can be slow for large datasets. Therefore, fitme tends to outer-optimize by default for large datasets, unless there is a non-trivial resid.model. The precise criteria for selection of default method by fitme are liable to future changes.

Further, the internal fitting methods of HLfit also provide some more information such as the "cond. SE" (about which see warning in Details of HLfit). To force the evaluation of such information after an outer-optimization by a fitme call, use the control\$refit argument (see Example). Alternatively (and possibly of limited use), one can force inner-optimization of lambda for a given random effect, or of phi, by setting it to NaN in init (see Example using 'blackcap' data). The same syntax may be tried for phi.

#### Value

The return value of an HLCor or an HLfit call, with additional attributes. The HLCor call is evaluated at the estimated correlation parameter values. These values are included in the return object as its \$corrPars member. The attributes added by fitme include the original call of the function (which can be retrived by getCall(<fitted object>), and information about the optimization call within fitme.

```
## Examples with Matern correlations
## A likelihood ratio test based on the ML fits of a full and of a null model.
 data("blackcap")
 (fullfit <- fitme(migStatus ~ means+ Matern(1|longitude+latitude),data=blackcap) )</pre>
 (nullfit <- fitme(migStatus ~ 1 + Matern(1|longitude+latitude),data=blackcap))</pre>
 ## p-value:
 1-pchisq(2*(logLik(fullfit)-logLik(nullfit)),df=1)
## See ?spaMM for examples of conditional autoregressive model and of non-spatial models.
## Contrasting different optimization methods:
# We simulate Gamma deviates with mean mu=3 and variance=2,
# ie. phi= var/mu^2= 2/9 in the (mu, phi) parametrization of a Gamma
# GLM; and shape=9/2, scale=2/3 in the parametrisation of rgamma().
# Note that phi is not equivalent to scale:
# shape = 1/phi and scale = mu*phi.
set.seed(123)
gr <- data.frame(y=rgamma(100,shape=9/2,scale=2/3))</pre>
# Here fitme uses HLfit methods which provide cond. SE for phi by default:
fitme(y~1,data=gr,family=Gamma(log))
# To force outer optimization of phi, use the init argument:
fitme(y~1,data=gr,family=Gamma(log),init=list(phi=1))
# To obtain cond. SE for phi after outer optimization, use the 'refit' control:
fitme(y~1,data=gr,family=Gamma(log),,init=list(phi=1),
      control=list(refit=list(phi=TRUE))) ## or ...refit=TRUE...
```

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fitmv

Fitting multivariate responses

# **Description**

This function extends the fitme function to fit a joint model for different responses (following possibly different response families) sharing some random-effects, including a new type of random effect defined to exhibit correlations across different responses (see mv). It is also possible to declare shared fixed-effect coefficients among different submodels, using the X2X argument. Only a few features available for analysis of univariate response may not yet work (see Details).

### Usage

#### **Arguments**

submodels

A list of sublists each specifying a model for each univariate response. The names given to each submodel in the main list are currently ignored. The names and syntax of elements within each sublist are those of a fitme call. In most cases, each sublist should not contain arguments whose names are those of formal arguments of fitmv itself (with the possible exception for fixed).

prior.weights (or better, weights.form), if any, should be specified as part of a submodel.

data

A data frame containing the variables in the response and the model formulas.

fixed

A list of fixed values of the parameters controlling random effects. The syntax is that of the same argument in fitme (the optional fixed argument in each sublist of submodels may also be used but this feature may be confusing). Fixed phi values must be specified as a list, e.g., fixed=list(phi=list("2"=0.1)) to set the value for the second submodel.

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init, lower, upper

Lists of initial values or bounds. The syntax is that of the same arguments in fitme. In these lists, random effects should be indexed according to their order of appearance in the total model (see Details). Any init, lower, or upper in a subject of submodel a will be invested.

sublist of submodels will be ignored.

control A list of control parameters, with possible elements as described for fitme

control.dist See control.dist in HLCor

method Character: the fitting method to be used, such as "ML", "REML" or "PQL/L".

"ML" is the default, as for fitme and in contrast to "REML" for the other fitting functions. Other possible values of HLfit's method argument are handled.

init. HLfit See identically named HLfit argument.

NULL, or a matrix **M** by which one can specify, as  $\beta = \mathbf{M}\beta^*$ , fixed effects  $\beta$ 

with some coefficients shared between submodels, e.g. as shown in the "Shared fixed effect" Example, where  $\beta^*$  has three distinct elements, and  $\beta$  has four elements including identical Intercept coefficients among the two submodels. The fixed-effect term  $\mathbf{X}\beta$  of the linear predictor thus takes the form  $\mathbf{X}\mathbf{M}\beta^*$ , meaning that the default design matrix of the model  $\mathbf{X}$  is replaced by  $\mathbf{X}\mathbf{M}$ .  $\mathbf{M}$ 

must have column names, labeling the  $\beta^*$  coefficients.

.. Optional arguments passed to (or operating as if passed to) HLCor, HLfit or

 $\verb|mat_sqrt|, for example control. HLf it or the covStruct, distMatrix, corrMatrix|$ 

or adjMatrix arguments of HLCor.

#### **Details**

### Matching random effects across submodels, and referring to them;

Random effects are recognized as identical across submodels by matching the formula terms. As shown in the Examples, if the two models formulas share the (1|clinic) term, this term is recognized as a single random effect shared between the two responses. But the (1|clinic) and (+1|clinic) terms are recognized as distinct random effects. In that case, the init argument init=list(lambda=c('1'=1,'2'=0.5)) is shown to refer to these by names 1,2... where the order is defined as the order of first appearance of the terms across the model formulas in the order of the submodels list. Alternatively, the syntax fixed=list(lambda=c('clinic.1'=0.5,'clinic'=1)) works: this syntax makes order of input irrelevant but assumes that the user guesses names correctly (these are typically the names that appear in the summary of lambda values from the fit object or, more programmatically,

names(<fit object>\$lambda.object\$print\_namesTerms)). Finally, fixed values of parameters can **also** be specified through each sub-model, with indices referring to the order of random effects with each model.

The matching of random-effect terms occurs after expansion of multIMRF terms, if any. This may have subtle consequences if two multIMRF terms differ only by their number of levels, as some of the expanded IMRF terms are then shared.

### **Capacities and limitations:**

Practically all features of models that can be fitted by fitme should be available: this includes all combinations of GLM response families, residual dispersion models, and all types of random-effect terms, whether autocorrelated or not. Among the arguments handled through the ..., covStruct, distMatrix, corrMatrix should be effective; control.HLfit\$LevenbergM and verbose=c(TRACE=TRUE) will work but some other controls available in fitme may not. Usage of the REMLformula argument

is restricted as it cannot be used to specify a non-standard REML correction (but the more useful keepInREML attribute for fixed fixed-effect coefficients is handled).

The multi family-like syntax for multinomial models should not be used, but fitmv could provide other means to model multinomial responses.

Most post-fit functions work, at least with default arguments. This includes point prediction and prediction variances calculations sensu lato, including with newdata; but also simulate, spaMM\_boot, confint, anova, update\_resp, and update. The re.form argument now works for predict and simulate. Bootstrap computation may require special care for models where simulation of one response variable may depend on draws of another one (see Hurdle model example in the "Gentle introdution" to spaMM, https://gitlab.mbb.univ-montp2.fr/francois/spamm-ref/-/blob/master/vignettePlus/spaMMintro.pdf).

Prediction functions try to handle most forms of missing information in newdata (including information missing for a residual-dispersion model when predictions fro mit are needed: see Examples). As information may be missing for some submodels but not others, different numbers of predictions are then returned for different submodels. As for univariate-response models, predict will return point predictions as a single 1-column matrix, here concatenating the prediction results of the different submodels. The nobs attribute specifies how may values pertain to each submodel.

Some plotting functions may fail. update.formula fails (see update\_formulas for details). terms returns a list, which is not usable by other base R functions. stats::step is a good example of resulting limitations, as it is currently unable to perform any sensible operation on fitmv output. spaMM::MSFDR which calls stats::step likewise fails. multcomp::glht fails.

A perhaps not entirely satisfying feature is that simulate by default stacks the results of simulating each submodel in a single vector. Some non-trivial reformatting may then be required to include such simulation results in a suitable newdata data frame with (say) sufficient information for prediction of all responses. The syntax

update\_resp(<fit>, newresp = simulate(<fit>, ...), evaluate = FALSE)\$data may be particularly useful to reformat simulation results in this perspective.

### Which arguments belong to submodels?:

Overall, arguments specifying individual submodels should go into submodels, while other arguments of fitmv should be those potentially affecting several submodels (notably, random-effect structures, lower, and upper) and fitting controls (such as init and init.HLfit). One rarely-used exception is REMLformula which controls the fitting method but should be specified through the submodels.

The function proceeds by first preprocessing all submodels independently, before merging the resulting information by matching random effects across submodels. The merging operation includes some checks of consistency across submodels, implying that redundant arguments may be needed across submodels (e.g. specifying twice a non-default rand.family for a random effect shared by two submodels).

#### Value

A (single) list of class HLfit, as returned by other fitting functions in **spaMM**. The main difference is that it contains a families element describing the response families, instead of the family elements of fitted objects for univariate response.

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#### See Also

See further examples in mv (modelling correlated random effects over the different submodels), and residVar

```
### Data preparation
data(clinics)
climv <- clinics</pre>
(fitClinics <- HLfit(cbind(npos,nneg)~treatment+(1|clinic),</pre>
                                             family=binomial(),data=clinics))
set.seed(123)
climv$np2 <- simulate(fitClinics, type="residual")</pre>
### fits
#### Shared random effect
(mvfit <- fitmv(</pre>
   submodels=list(mod1=list(formula=cbind(npos,nneg) \\ ~treatment+(1|clinic),family=binomial()),\\ ~treatment+(1|
                                      mod2=list(formula=np2~treatment+(1|clinic),
                                                            family=poisson(), fixed=list(lambda=c("1"=1)))),
      data=climv))
# Two univariate-response independent fits because random effect terms are distinct
# (note how two lambda values are set; same syntax for 'init' values):
(mvfitind <- fitmv(</pre>
   submodels=list(mod1=list(formula=cbind(npos,nneg)~treatment+(1|clinic),family=binomial()),
                                      mod2=list(formula=np2~treatment+(+1|clinic),family=poisson())),
      data=climv, fixed=list(lambda=c('1'=1,'2'=0.5)))) # '1': (1|clinic); '2': (+1|clinic)
#### Specifying fixed (but not init) values in submodels is also possible (maybe not a good idea)
# (mvfitfix <- fitmv(</pre>
        submodels=list(mod1=list(formula=cbind(npos,nneg)~treatment+(1|clinic),
                                                  family=binomial(),fixed=list(lambda=c('1'=1))), # '1': (1|clinic)
#
                                        mod2=list(formula=np2~treatment+(+1|clinic),family=poisson(),
                                                       fixed=list(lambda=c('1'=0.5))),
#
                                                                                                                                                   # '2': (+1|clinic)
#
        data=climv))
#### Shared fixed effect
# Suppose we want to fit the same intercept for the two submodels
# (there may be cases where this is meaningful, even if not here).
# The original fit has four coefficients corresponding to four columns
# of fixed-effect design matrix:
head(design_X <- model.matrix(mvfit))</pre>
# (Intercept)_1 treatment_1 (Intercept)_2 treatment_2
# [1,]
              . . .
# The three coefficients of the intended model are (say)
# "(Intercept)" "treatment_1" "treatment_2"
# We build a matrix that relates the original 4 coefficients to these 3 ones:
```

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```
X_4to3 <-
  matrix(c(1,0,0,
           0,1,0,
           1,0,0,
           0,0,1), nrow=4, ncol=3, byrow=TRUE,
         dimnames=list(NULL, c("(Intercept)", "treatment_1", "treatment_2")))
# defined such that design_X %*% X_4to3 will be the design matrix for the intended model,
# and the single "(Intercept)" coefficient of the three-parameter model will operate as
# a shared estimate of the "(Intercept)_1" and "(Intercept)_2" coefficients
# of the original 4-coefficients model, as intended.
# To define such matrices, it is *strongly advised* to fit the unconstrained model first,
# and to examine the structure of its model matrix (as shown above).
# The new fit is obtained by providing the matrix as the 'X2X' argument:
(mvfit3 <- fitmv(
  submodels=list(mod1=list(formula=cbind(npos,nneg)~treatment+(1|clinic),family=binomial()),
                   mod2=list(formula=np2~treatment+(1|clinic),
                             family=poisson(), fixed=list(lambda=c("1"=1)))),
    X2X = X_4to3
    data=climv))
\# => the column names of 'X_4to3' are the fixed-effect names in all output.
#### Prediction with a residual-dispersion model
set.seed(123)
beta_dat <- data.frame(y=runif(100),grp=sample(2,100,replace = TRUE), x_het=runif(100),</pre>
                       y2=runif(100))
(mvfit <- fitmv(list(list(y ~1+(1|grp), family=beta_resp(), resid.model = ~x_het),</pre>
                   list(y2 ~1+(1|grp), family=beta_resp())),
              data= beta_dat))
misspred <- beta_dat[1:3,]</pre>
misspred$x_het[1] <- NA # missing info for residual variance of first submodel
## => prediction missing when this info is needed:
#
length(predict(mvfit, newdata=misspred)) # 6 values: missing info not needed for point predictions
length(get_residVar(mvfit, newdata=misspred)) # 5 values
length(get_respVar(mvfit, newdata=misspred)) # 5 values
# Missing info not needed for predVar (**as opposed to respVar**)
length(get_predVar(mvfit, newdata=misspred)) # 6 values
# Same logic for interval computations:
dim(attr(predict(mvfit, newdata=misspred, intervals="respVar"), "intervals")) # 5,2
dim(attr(predict(mvfit, newdata=misspred, intervals="predVar"), "intervals")) # 6,2
# Same logic for simulate():
```

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length(simulate(mvfit, newdata=misspred)) # 5 as simulation requires residVar

fixed

Fixing some parameters

# Description

The fitting functions allow all parameters to be fixed rather than estimated:

- \* Fixed-effect coefficients can be set by way of the etaFix argument (linear predictor coefficients) for all fitting functions.
- \* Random-effect parameters and the phi parameter of the gaussian and Gamma response families can be set for all fitting function by the fixed argument, or for some fitting functions by an alternative argument with the same effect (see Details for this confusing feature, but using fixed uniformly is simpler).
- \* The ad-hoc dispersion parameter of some response families (COMPoisson, negbin1, negbin2, beta\_resp, betabin and possibly future ones) can be fixed using the ad-hoc argument of such families rather than by fixed.

#### **Details**

etaFix is a list with single documented element beta, which should be a vector of (a subset of) the coefficients ( $\beta$ ) of the fixed effects, with names as shown in a fit without such given values. If REML is used to fit random effect parameters, then etaFix affects by default the REML correction for estimation of dispersion parameters, which depends only on which  $\beta$  coefficients are estimated rather than given. This default behaviour will be overridden whenever a non-null REML formula is provided to the fitting functions (see Example). Alternatively, with a non-NULL etaFix\$beta, REML can also be performed as if all  $\beta$  coefficients were estimated, by adding attribute keepInREML=TRUE to etaFix\$beta; in that case the REML computation is by default that implied by the fixed effects in the full model formula, unless a non-default REML formula is also used.

The older equivalent for the fixed argument is ranFix for HLfit and corrHLfit, and ranPars for HLCor. Do not use both one such argument and fixed in a call. This older diversity of names was confusing, but its logic was that ranFix allows one to fix parameters that HLfit and corrHLfit would otherwise estimate, while ranPars can be used to set correlation parameters that HLCor does not estimate but nevertheless requires (e.g., Matérn parameters).

Theses arguments for fixing random-effect parameters all have a common syntax. They is a list, with the following possible elements, whose nature is further detailed below:

- \* phi (variance of residual error, for gaussian and Gamma HGLMs),
- \* lambda (random-effect variances, except for random-coefficient terms),
- \* ranCoefs (random-coefficient parameters),
- \* corrPars (correlation parameters, when handled by the fitting function).
- \* Individual correlation parameters such as **rho**, **nu**, **Nugget**, **ARphi**... are also possible top-level elements of the list when there is no ambiguity as to which random effect these correlation parameters apply. This syntax was conceived when spaMM handled a single spatial random effect, and it is still convenient when applicable, but it should not be mixed with corrPars element usage.

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**phi** may be a single value or a vector of the same length as the response vector (the number of rows in the data, once non-informative rows are removed).

lambda may be a single value (if there is a single random effect, or a vector allowing to specify unambiguously variance values for some random effect(s). It can thus take the form lambda=c(NA, 1) or lambda=c("2"=1) (note the name) to assign a value only to the variance of the second of two random effects.

ranCoefs is a list of numeric vectors, each numeric vector specifying the variance and correlation parameters for a random-coefficient term. As for lambda, it may be incomplete, using names to specify the random effect to which the parameters apply. For example, to assign variances values 3 and 7, and correlation value -0.05, to the second random effect in a model formula, one can use ranCoefs=list("2"=c(3,-0.05,7)) (note the name). The elements of each vector are variances and correlations, matching those of the printed summary of a fit. The order of these elements must be the order of the lower. tri of a covariance matrix, as shown e.g. by

```
m2 <- matrix(NA, ncol=2,nrow=2); m2[lower.tri(m2,diag=TRUE)] <- seq(3); m2.</pre>
```

fitme accepts partially fixed parameters for a random coefficient term, e.g.,

ranCoefs=list("2"=c(NA,-0.05,NA)), although this may not mix well with some obscure options, such as

control=list(refit=list(ranCoefs=TRUE)) which will ignore the fixed values. GxE shows how to use partially-fixed ranCoefs to fit different variances for different levels of a factor.

corrPars is a list, and it may also be incomplete, using names to specify the affected random effect as shown for lambda and ranCoefs. For example, ranFix=list(corrPars=list("1"=list(nu=0.5))) makes explicit that nu=0.5 applies to the first ("1") random effect in the model formula. Its elements may be the correlation parameters of the given random effect. For the Matérn model, these are the correlation parameters rho (scale parameter(s)), nu (smoothness parameter), and (optionally) Nugget (see Matern). The rho parameter can itself be a vector with different values for different geographic coordinates. For the adjacency model, the only correlation parameter is a scalar rho (see adjacency). For the AR1 model, the only correlation parameter is a scalar ARphi (see AR1). Consult the documentation for other types of random effects, such as Cauchy or IMRF, for any information missing here.

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```
# so simply fixing the coefficients to their REML estimates will not yield
# the same REML fits, as see by comparing the next two fits:
unconstr < fitme(y \sim X1+X2+X1*X3+X2*X3+I(X2^2)+(1|batch), data=wafers,
                  family=Gamma(log), method="REML")
# Second fit is different from 'unconstr' despite the same fixed-effects:
naive <- fitme(y ^{X1+X2+X1*X3+X2*X3+I}(X2^2)+(1|batch), data=wafers, family=Gamma(log),
               method="REML", etaFix=list(beta=fixef(unconstr)))
# Using REMLformula to obtain the same REML fit as the unconstrained one:
fitme(y \sim X1+X2+X1*X3+X2*X3+I(X2^2)+(1|batch), data=wafers, family=Gamma(log),
      method="REML", etaFix=list(beta=fixef(unconstr)),
      REMLformula=y ~X1+X2+X1*X3+X2*X3+I(X2^2)+(1|batch))
data("Loaloa")
# Fixing some Matern correlation parameters, in fitme():
fitme(cbind(npos,ntot-npos) ~ elev1 +Matern(1|longitude+latitude),
             data=Loaloa,family=binomial(),fixed=list(nu=0.5,Nugget=2/7))
# Fixing all mandatory Matern correlation parameters, in HLCor():
HLCor(cbind(npos,ntot-npos) ~ elev1 + Matern(1|longitude+latitude),
             data=Loaloa,family=binomial(),ranPars=list(nu=0.5,rho=0.7))
## End(Not run)
```

fixedLRT

Likelihood ratio test of fixed effects.

### Description

fixedLRT performs a likelihood ratio (LR) test between two models, the "full" and the "null" models, currently differing only in their fixed effects. Parametric bootstrap p-values can be computed, either using the raw bootstrap distribution of the likelihood ratio, or a bootstrap estimate of the Bartlett correction of the LR statistic. This function differs from LRT in its arguments (model fits for LRT, versus all arguments required to fit the models for fixedLRT), and in the format of its return value.

## Usage

```
fixedLRT(null.formula, formula, data, method, HLmethod = method,
    REMLformula = NULL, boot.repl=0, control="DEPRECATED",
    control.boot="DEPRECATED", fittingFunction, seed=NULL,
    resp_testfn = NULL, weights.form = NULL, ...)
```

#### **Arguments**

null. formula Either a formula (as in glm) or a predictor (see Predictor) for the null model.

Either a formula or a predictor for the full model.

A data frame containing the variables in the model.

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method A method to fit the full and null models. See method information about such

methods. The two most meaningful values of method in fixedLRT calls are: 'ML' for an LRT based on ML fits (generally recommended); and 'PQL/L' for

an LRT based on PQL/L fits (recommended for spatial binary data).

Also feasible, but more tricky, and not really recommended (see Rousset and Ferdy, 2014), is 'REML'. This will perform an LRT based on two REML fits of the data, \*both\* of which use the same conditional (or "restricted") likelihood of residuals for estimating dispersion parameters  $\lambda$  and  $\phi$  (see REMLformula argument). Further, REML will not be effective on a given dispersion parameter

if a non-trivial init.corrHLfit value is provided for this parameter.

HLmethod Kept for back-compatibility. Same as method, but may work only for

fittingFunction=corrHLfit.

REMLformula a formula specifying the fixed effects which design matrix is used in the REML

correction for the estimation of dispersion parameters, if these are estimated by

REML. This formula is by default that for the \*full\* model.

weights.form Specification of prior weights by a one-sided formula: use weights.form = ~

pw instead of prior.weights = pw. The effect will be the same except that such an argument, known to evaluate to an object of class "formula", is suitable to

enforce safe programming practices (see good-practice).

boot.repl the number of bootstrap replicates.

control Deprecated. control.boot Deprecated.

fittingFunction

Character string giving the function used to fit each model: either "corrHLfit" or "fitme". Default is "corrHLfit" for small data sets (fewer than 300 observations), and "fitme" otherwise, but this may change in future versions.

seed Passed to simulate. HLfit

resp\_testfn See argument resp\_testfn of spaMM\_boot

... Further arguments passed to or from other methods; presently, additional argu-

ments passed to fitting functions.

### **Details**

Comparison of REML fits is a priori not suitable for performing likelihood ratio tests. Nevertheless, it is possible to contrive them for testing purposes (Welham & Thompson 1997). This function generalizes some of Wehlam & Thompson's methods to GLMMs.

See Details in LRT for details of the bootstrap procedures.

#### Value

An object of class fixedLRT, actually a list with as-yet unstable format, but here with typical elements (depending on the options)

fullfit the HLfit object for the full model; nullfit the HLfit object for the null model; 80 fix\_predVar

LRTori A likelihood ratio chi-square statistic

LRTprof Another likelihood ratio chi-square statistic, after a profiling step, if any.

df the number of degrees of freedom of the test.

trace.info Information on various steps of the computation.

and, if a bootstrap was performed, the additional elements described in LRT.

#### References

Rousset F., Ferdy, J.-B. (2014) Testing environmental and genetic effects in the presence of spatial autocorrelation. Ecography, 37: 781-790. doi:10.1111/ecog.00566

Welham, S. J., and Thompson, R. (1997) Likelihood ratio tests for fixed model terms using residual maximum likelihood, J. R. Stat. Soc. B 59, 701-714.

#### See Also

See LRT for simular tests with a different interface, and perhaps as\_LMLT for access to a different testing approach for LMMs, implemented in lmerTest::contest.

### **Examples**

fix\_predVar

Prediction from models with nearly-singular covariance matrices

### **Description**

This explains how to handle a warning occurring in computation of prediction variance, where the user is directed here.

For **Matern or Cauchy** correlation models with vanishing scale factor for distances, a warning may be produced when predict.HLfit (or get\_predVar, etc.) is called with non-NULL newdata, because a nearly-singular correlation matrix of the random effect is met. **To decide what to do** in that case, users should compare the values of get\_predVar(.) and get\_predVar(., newdata=myfit\$data) (see Example below). In the absence of numerical inaccuracies, The two

fix\_predVar 81

values should be identical, and in the presence of such inaccuracies, the more reliable value is the first one. In really poor cases, the second syntax may yield negative prediction variances. If users deem the inaccuracies too large, they should use control=list(fix\_predVar=TRUE) in the next call to predict.HLfit (or get\_predVar, etc.) as shown in the Example. The drawback of this control is that the computation may be slower, and might even exceed memory capacity for large problems (some matrix operations being performed with exact rational arithmetic, which is memory-consuming for large matrices). it is also still experimental, in the sense that I fear that bugs (stop) may occur. If the user instead chooses control=list(fix\_predVar=FALSE), the default standard floating-point arithmetic is used, but no warning is issued.

For fix\_predVar left NULL (the default), standard floating-point arithmetic is also used. But in addition (with exceptions: see Details), the warning keeps being issued, and the (possibly costly) computation of the inverse of the correlation matrix is not stored in the fitted model object, hence is repeated for each new prediction variance computation. This is useful to remind users that something needs to be done, but for programming purposes where repeated warnings may be a nuisance, one can use control=list(fix\_predVar=NA) which will issue a warning then perform as control=list(fix\_predVar=FALSE), i.e. store an approximate inverse so the warning is not issued again. Finally, control=list(fix\_predVar=NaN) will remove the inverse of the correlation matrix from the fitted model object, and start afresh as if the control was NULL.

#### **Details**

Nearly-singular correlation matrices of random effects occur in several contexts. For random-slope models, it commonly occurs that the fitted correlation between the random effects for Intercept and slope is 1 or -1, in which case the correlation matrix between these random effects is singular. This led to quite inaccurate computations of prediction variances in spaMM prior to version 3.1.0, but this problem has been fixed.

control=list(fix\_predVar=NaN) may be more appropriate than control=list(fix\_predVar=NULL) when predict.HLfit is called through code that one cannot control. For this reason, spaMM provides another mode of control of the default. It will convert control=list(fix\_predVar=NULL) to other values when the call stack has call names matching the patterns given by spaMM.getOption("fix\_predVar") (as understood by grep). Thus if spaMM.getOption("fix\_predVar")\$"NA"=="MSL|b the default behaviour is that defined by control=list(fix\_predVar=NA) when predict.HLfit is called through Infusion::MSL or blackbox::bboptim. FALSE or TRUE are handled in a similar way.

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freight

Freight dataset

# Description

A set of data on airfreight breakage. Data are given on 10 air shipments, each carrying 1000 ampules of some substance. For each shipment, the number of ampules found broken upon arrival, and the number of times the shipments were transferred from one aircraft to another, are recorded.

# Usage

```
data("freight")
```

### **Format**

The data frame includes 10 observations on the following variables:

broken number of ampules found broken upon arrival.

transfers number of times the shipments were transferred from one aircraft to another.

id Shipment identifier.

### **Source**

The data set is reported by Kutner et al. (2003) and used by Sellers & Shmueli (2010) to illustrate COMPoisson analyses.

# References

Kutner MH, Nachtsheim CJ, Neter J, Li W (2005, p. 35). Applied Linear Regression Models, Fourth Edition. McGraw-Hill.

Sellers KF, Shmueli G (2010) A Flexible Regression Model for Count Data. Ann. Appl. Stat. 4: 943–961

```
## see ?COMPoisson for examples
```

get\_cPredVar 83

get_cPredVar	Estimation of prediction variance with bootstrap correction

### **Description**

This function is similar to get\_predVar except that is uses a bootstrap procedure to correct for bias in the evaluation of the prediction variance.

### Usage

# Arguments

pred_object	an object of class HLfit, as returned by the fitting functions in spaMM.
newdata	passed to predict. HLfit (it thus represents a prediction design, not to be confused with the bootstrap samples)
nsim	passed to simulate.HLfit
seed	passed to simulate.HLfit
type	passed to simulate.HLfit
variances	NULL or list; variances["cov"] will be passed to predict.HLfit to control whether a covariance matrix is computed or not. Other elements are currently ignored.
nb_cores	integer: number of cores to use for parallel computation of bootstrap. The default is spaMM.getOption("nb_cores"), and 1 if the latter is NULL.nb_cores=1 prevents the use of parallelisation procedures.
fit_env	For parallel computations: an environment containing objects to be passed to the cores. They should have the same name in fit_env as in the environment they are passed from.
sim_object	an object of class HLfit, passed to simulate.HLfit as its object argument. Simulating from this object must produce response values that can be used as replacement to those of the original fitted pred_object. In standard usage, sim_object=pred_object (the default).

### **Details**

The result provided by get\_cPredVar is similar to the CMSEP (Conditional Mean Standard Error of Prediction) introduced by Booth and Hobert (1998; "B&H"). This paper is known for pointing the importance of using conditional variances when they differ from unconditional ones. This is hard to miss in spatial models, where the relevant prediction variance typically depends on the variance of random effects conditional on the data. Thus, the alternative function get\_predVar already accounts for this and returns a prediction variance that depends on a joint covariance of fixed-effect estimates and of random effects given the data.

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B&H also used a conditional bootstrap procedure to correct for some bias. get\_cPredVar implements a similar procedure, in contrast to get\_predVar. Their conditional bootstrap procedure is not applicable for autocorrelated random effects, and parametric bootstrapping of the residuals of the fitted model (as implied by the default value of argument type) is used instead here. Apart from this difference, the returned value includes exactly the same terms as those discussed by B&H: their "naive estimate"  $\nu_i$  and its bootstrap correction  $b_i$ , their correction  $\beta$  for uncertainty in fixed-effect coefficients, and their correction  $\sigma^2$  for uncertainty in dispersion parameters.

This use of the bootstrap does not account for uncertainty in correlation parameters "outer-optimized" by fitme or corrHLfit, because the correlation parameters are fixed when the model is refitted on the bootstrap replicates. Even if it the correlation parameters were refitted, the full computation would not be sufficient to account for uncertainty in them. To account for uncertainty in correlation parameters, one should rather perform a parametric bootstrap of the full model (typically using spaMM\_boot(., type="residual")), which may take much more time.

The "naive estimate"  $\nu_i$  is not generally an estimate of anything uniquely defined by the model parameters: for correlated random effects, it depends on the "root" of the correlation matrix of the random effects, which is not unique. Thus  $\nu_i$  is not unique, and may differ for example for equivalent fits by sparse-precision methods vs. other methods. Nevertheless, attr(cpredvar, "info")n ve does recover published values in the Examples below, as they involve no correlation matrix.

#### Value

A vector of prediction variances, with an attribute info which is an **environment** containing variables:

SEs the standard errors of the estimates (which are those of the bootstrap replicates)

bias the bias term maive B&H's "naive"  $u_i$ 

### References

Booth, J.G., Hobert, J.P. (1998) Standard errors of prediction in generalized linear mixed models. J. Am. Stat. Assoc. 93: 262-272.

get\_inits\_from\_fit 85

get\_inits\_from\_fit

Initiate a fit from another fit

# **Description**

get\_inits\_from\_fit is an extractor of some fitted values from a fit in a convenient format to initiate a next fit.

# Usage

```
get_inits_from_fit(from, template = NULL, to_fn = NULL, inner_lambdas=FALSE)
```

# Arguments

from	Fit object (inheriting from class "HLfit") from which fitted values are taken.
template	Another fit object. Usage with a template fit object is suitable for refitting this object using fitted values from the from object as starting values.
to_fn	NULL or character: the name of the function to be used the next fit. If NULL, taken from template (if available), else from from. It is meaningful to provide a to_fn distinct from the function used to fit a template.
inner_lambdas	Boolean; Whether the output should include estimates of the dispersion parameters estimated by the iterative methods implemented in HLfit.

## Value

A list with elements

init, init.corrHLfit

(depending on the fitting function) giving initial values for outer-optimization;

init.HLfit giving in

giving initial values for the iterative algorithms in HLfit. It is itself a list with possible elements:

fixef for the coefficients of the linear predictor, adjusted to the format of the coefficients of the linear predictor of the template object, if available; ranCoefs random-coefficients parameters (if **not** outer-optimized).

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### See Also

```
get_ranPars and VarCorr.
```

### **Examples**

get\_matrix

Extract matrices from a fit

### **Description**

get\_matrix is a first attempt at a unified extractor of various matrices from a fit. All augmented matrices follow (Henderson's) block order (upper blocks: X,Z; lower blocks: 0,I). get\_ZALMatrix returns the design matrix for the random effects v.

## Usage

```
get_matrix(object, which="model.matrix", augmented=TRUE, ...)
get_ZALMatrix(object, force_bind=TRUE)
```

### **Arguments**

object

An object of class HLfit, as returned by the fitting functions in spaMM.

augmented

Boolean; whether to return a matrix for all model coefficients (augmented matrix for fixed-effects coefficients and random-effect predictions) or a matrix only for fixed effects. Not operative for all which values (currently only for which="left\_ginv").

which

Which element to extract. For "model.matrix", the design matrix for fixed effects (similarly to stats::model.matrix); for "ZAL", the design matrix for random effects (same as get\_ZALMatrix()), while "ZA" and "L" may return these two factors (detailed in random-effects); for "AugX", the (unweighted) augmented design matrix of the least-square problem; for "hat\_matrix", the projection matrix that gives model predictions from the (augmented) response

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vector; for "left\_ginv", the pseudo-inverse that gives the model coefficients from the (augmented) response vector. See Details for further definitions and options for functions of the augmented design matrix.

force\_bind

Boolean; with the non-default value FALSE, the function may return an object of class ZAXlist, which is poorly documented and for development purposes only.

... Other arguments that may be needed in some future versions of spaMM.

#### **Details**

(Given the pain that it is to write maths in R documentation files, readers are gently asked to be tolerant about any imperfections of the following).

Model coefficients estimates of a (weighted) linear model can be written as  $(X'WX)^{-1}X'Wy$  where **X** is the design matrix for fixed effects, **W** a diagonal weight matrix, and **y** the response vector. In a linear mixed model, the same expression holds in terms of Henderson's augmented design matrix, of an augmented (still diagonal) weight matrix, and of an augmented response vector. For GLMMs and hierarchical GLMs generally, the solution of each step of the iteratively reweighted least squares algorithm again has the same expression in terms of appropriately defined augmented matrices and vectors.

get\_matrix returns, for given values of the which argument, the following matrices from the model fir:

```
"AugX": X;
```

"wei\_AugX": WX;

"wAugX":  $\sqrt{(\mathbf{W})\mathbf{X}}$ ;

"left\_ginv":  $(X'WX)^{-1}X'W$  (the name stems from the fact that it is generalized inverse, denoted  $X^-$ , since  $XX^-X=X$ , and it is a left one, since  $X^-X$  is an identity matrix when X has full rank);

"hat\_matrix":  $XX^-=X(X'WX)^{-1}X'W$ ;

"fixef\_left\_ginv": same as "left\_ginv" but for the fixed-effect design matrix only (not to be confused with the corresponding block of "left\_ginv");

"beta\_v\_cov": joint covariance matrix of estimates/predictions of fixed-effect coefficients and random effects (the  $\mathbf{v}$  in random-effects). "v\_condcov": covariance matrix of predictions of random effects (the  $\mathbf{v}$  in random-effects) given fixed-effect coefficients.

## Value

A matrix, possibly in sparseMatrix format.

#### See Also

vcov for the variance-covariance matrix of the fixed-effects coefficients, and Corr for correlation matrices of random effects.

88 get\_ranPars

|--|

### Description

get\_fittedPars returns estimated parameters.

get\_ranPars returns various subsets of random-effect parameters (correlation or variance parameters), as controlled by its which argument. It is one of several extractors for fixed or estimated parameters of different classes of parameters, for which a quick guide is

get\_ranPars: for random-effect parameters, excluding residual dispersion (with a subtlety for corrFamily models: see Details);

VarCorr: alternative extractor for random-effect (co)variance and optionally residual variance, in a data frame format;

residVar: for residual variance parameters, family dispersion parameters, or information about residual variance models;

get\_residVar: alternative extractor of residual variances with different features inherited from get\_predVar;

get\_inits\_from\_fit: extracts estimated parameters from a fit, in a different format from get\_fittedPars.

remove\_from\_parlist removes elements from a list of parameters, and from its type attribute.

# Usage

# Arguments

object	An object of class HLfit, as returned by the fitting functions in spaMM.
partial_rC	Controls handling of partially-fixed random coefficients. The default as set by "rm" is to remove the fixed values as for other parameters. But alternative option "keep" will keep the fixed value, and NA will replace it by a NA.
phiPars	Boolean: whether to include the parameters of any residual-dispersion model for $phi$ (se phi-resid.model) in the rdisPars element of the returned list.
which	NULL or character string. Use which="corrPars" to get the correlation parameters. Use which="lambda" to get variances. see Details for the meaning of this for heteroscedastic models, and Value for other possible which values.
	Other arguments that may be needed by some method.
verbose	Boolean: Whether to print some notes.
parlist	A list of parameters. see Details.
removand	Optional. A list of parameters to be removed from parlist.

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rm\_names Names of parameters to be removed from parlist. Mandatory if removand is

not given.

lambda\_names By default the names of the lambda vector are built from the Group (RHS of

random effect term of the for (LHSIRHS)) and Term (variable from LHS). By setting a non-default value of lambda\_names the names will be integer indices of the random-effect term in the model formula (currently, for which="ranef\_var"

or NULL.

#### **Details**

For heteroscedastic random effects, such as conditional autoregressive models, the variance parameter "lambda" refers to a common scaling coefficient. For other random-effect models, "lambda" typically refers to the single variance parameter.

remove\_from\_parlist is designed to manipulate structured lists of parameters, such as a list with elements phi, lambda, and corrPars, the latter being itself a list structured as the return value of get\_ranPars(.,which="corrPars"). parlist may have an attribute type, also with elements phi, lambda, and corrPars... If given, removand must have the same structure (but typically not all the elements of parlist); otherwise, rm\_names must have elements which match names of unlist(names(parlist)).

If a corrFamily parameter is fixed through the formula term, as in ARp(1|time, p=3, fixed=c(p2=0)), the fixed parameter is not considered a model parameter and get\_ranPars will not extract it from the object. However, the parameter will be extracted if it has been fixed through fitme's fixed argument rather than through the formula term (see example in ARp).

### Value

get\_fittedPars returns a list of model parameters, with possible elements: beta (fixed-effect coefficients); lambda, phi, ranCoefs and corrPars (same meaning as in fixed parameters); hyper, for multIMRF models; the residual-dispersion parameters beta\_prec, NB\_shape and COMP\_nu when they are single scalars; and rdisPars for more complex residual-dispersion parameters. See the specific resid.model and phi-resid.model documentations for the rdisPars format, dependent on the nature of the residual-dispersion parameter being modelized. Use residVar(., which="fam\_parm") to extract the vector of fitted values of the dispersion parameter.

get\_ranPars(.,which="corrPars") returns a (possibly nested) list of correlation parameters (or NULL if there is no such parameter). Top-level elements correspond to the different random effects. The list has a "type" attribute having the same nested-list structure and describing whether and how the parameters where fitted: "fix" means they where fixed, not fitted; "var" means they were fitted by HLfit's specific algorithms; "outer" means they were fitted by a generic optimization method.

get\_ranPars(.,which="lambda") returns a vector of variance values, one per random effect, including both fixed, "outer"- and "inner"-optimized ones. The variances of random-coefficients terms with correlation parameters are not included.

get\_ranPars(.,which="outer\_lambda") returns only "outer"-optimized variance parameters,
ignoring those fitted by HLfit's specific algorithms.

get\_ranPars(., which=NULL) (the default) is not fully defined. It returns a list including the results of which="lambda" and which="corrPars", but possibly other elements too.

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get\_ranPars(.,which="fitted") is designed to provide fitted parameters with respect to which an information matrix is to be calculated (using **numDeriv**. It excludes fixed values, and has no type attribute.

```
get_ranPars(. which="ranef_var") (experimental) returns a list with elements
Var same as get_ranPars(.,which="lambda")
lembda_est A vector of variance values, one for each level of each random effect
outer A vector or outer-optimized variance values, as returned by get_ranPars(.,which="outer_lambda")
... Other elements, subject to change in later versions.
```

remove\_from\_parlist returns a list of model parameters with given elements removed, and likewise for its (optional) type attribute. See Details for context of application.

#### See Also

See get\_fittedPars, VarCorr, residVar, get\_residVar, or get\_inits\_from\_fit as described in the quick guide above.

### **Examples**

```
data("wafers")
m1 <- HLfit(y ~X1+X2+(1|batch), resid.model = ~ 1, data=wafers, method="ML")
get_ranPars(m1,which="corrPars") # NULL since no correlated random effect

parlist1 <- list(lambda=1,phi=2,corrPars=list("1"=list(rho=3,nu=4),"2"=list(rho=5)))
parlist2 <- list(lambda=NA,corrPars=list("1"=list(rho=NA))) # values of elements do not matter
remove_from_parlist(parlist1,parlist2) ## same result as:
remove_from_parlist(parlist1,rm_names = names(unlist(parlist2)))</pre>
```

get\_RLRsim\_args

Extractors of arguments for functions from package RLRsim

### **Description**

get\_RLRsim\_args extracts a list of arguments suitable for a call to RLRsim::RLRTSim() or RLRsim::LRTSim(). These functions use an efficient simulation procedure to compute restricted or marginal likelihood ratio tests, respectively, comparing a fixed-effect model and a mixed-effect model with one random effect. They are notably used to test for the presence of one random effect, although the models compared by marginal likelihood (LRTSim()) may differ both in their random and in their fixed effects (as shown in the Example). The tests are exact for small samples (up to simulation error) for LMMs with no free parameters in the random effect (beyond the variance being tested), so not for time-series or spatial models with estimated correlation parameters. Heteroscedasticity of the residuals or of the random effect variance are also not taken into account by the simulation procedure (see Value field below for an hint why this is so).

get\_RLRTSim\_args is the older extractor, originally for RLRsim::RLRTSim() only, now handling also ML fits with a warning (though the possible absence of the nullfit argument will result in an error).

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#### Usage

```
get_RLRsim_args(fullfit, nullfit, verbose=TRUE, REML=NA, ...)
get_RLRTSim_args(object, verbose=TRUE, ...)
```

### **Arguments**

object, fullfit An object of class HLfit, as returned by the fitting functions in spaMM, for the more complete model to be compared.

nullfit Same for the less complete model; required only for (marginal) LR test, as opposed to restricted LR test.

verbose NA or boolean; Whether to display some message or not.

REML For programming purposes, not documented.

... Additional arguments (currently not used).

#### **Details**

If the models compared do not differ in their fixed effects, under the null hypothesis there is a probability mass P for a zero likelihood ratio, and the distribution of p-values can be uniform only on the range (0,1-P). If the fixed effects differ (as handled by RLRsim::LRTSim()), this does not occur.

### Value

A list of arguments for a call to RLRsim::RLRTSim() or RLRsim::LRTSim(). The main arguments are the design matrix for the fixed effects, and the **ZA** matrix and **L** detailed in random-effects (here represented by the Z and sqrt.Sigma elements). The models handled by the testing procedure are the ones that are sufficiently characterized by these two matrices. LRTSim additionally requires q, the difference in number of parameters of fixed effects between the models.

### Note

The inconsistent capitalisation of 's' in the function names is consistent with the inconsistencies in the RLRsim package.

### References

Crainiceanu, C. and Ruppert, D. (2004) Likelihood ratio tests in linear mixed models with one variance component, *Journal of the Royal Statistical Society: Series B*,**66**,165–185.

#### See Also

The bootstrap procedure in LRT is more general but slower. It appears to provide results quite similar to those of RLRsim when both are applicable.

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### **Examples**

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Clear and trustworthy formulas and prior weights

### **Description**

Base fitting functions in R will seek variables in the environment where the formula was defined (i.e., typically in the global environment), if they are not in the data. This increases the memory size of fit objects (as the formula and attached environment are part of such objects). This also easily leads to errors (see example in the discussion of update.HLfit). Indeed Chambers (2008, p.221), after describing how the environment is defined, comments that "Where clear and trustworthy software is a priority, I would personally avoid such tricks. Ideally, all the variables in the model frame should come from an explicit, verifiable data source...". Fitting functions in **spaMM** try to adhere to such a principle, as they assume by default that all variables from the formula should be in the data argument (and then, **one never needs to specify** "data\$" in the formula.. **spaMM** implements this by default by stripping the formula environment from any variable. It is also possible to assign a given environment to the formula, through the control control.HLfit\$formula\_env: see Examples.

The variables defining the prior.weights should also be in the data. However, the implementation of the prior.weights argument has limitations that can be overcome by using the more recently introduced weights.formula argument of **spaMM** fitting functions (see Examples, where this is also compared with stats::lm's handling of its weights argument).

However, variables used in other arguments such as ranFix are looked up neither in the data nor in the formula environment, but in the calling environment as usual.

#### References

Chambers J.M. (2008) Software for data analysis: Programming with R. Springer-Verlag New York

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```
###### Controlling the formula environment
set.seed(123)
d2 \leftarrow data.frame(y = seq(10)/2+rnorm(5)[gl(5,2)], x1 = sample(10), grp=gl(5,2), seq10=seq(10))
# Using only variables in the data: basic usage
# HLfit(y \sim x1 + seq10+(1|grp), data = d2)
# is practically equivalent to
HLfit(y \sim x1 + seq10+(1|grp), data = d2,
      control.HLfit = list(formula_env=list2env(list(data=d2))))
# The 'formula_env' avoids the need for the 'seq10' variable:
HLfit(y \sim x1 + I(seq\_len(nrow(data))) + (1|grp), data = d2,
      control.HLfit = list(formula_env=list2env(list(data=d2))))
# Internal imprementation exploits partial matching of argument names
# so that this can also be in 'control' if 'control.HLfit' is absent:
fitme(y \sim x1 + I(seq\_len(nrow(data))) + (1|grp), data = d2,
      control = list(formula_env=list2env(list(data=d2))))
###### Prior-weights misery
data("hills", package="MASS")
(fit <- lm(time ~ dist + climb, data = hills, weights=1/dist^2))</pre>
# same as
(fit <- fitme(time ~ dist + climb, data = hills, prior.weights=1/dist^2, method="REML"))
# possible calls:
(fit <- fitme(time ~ dist + climb, data = hills, prior.weights=quote(1/dist^2)))</pre>
(fit <- fitme(time ~ dist + climb, data = hills, prior.weights= 1/hills$dist^2))</pre>
(fit <- fitme(time ~ dist + climb, data = hills, weights.form= ~ 1/dist^2))
(fit <- fitme(time ~ dist + climb, data = hills, weights.form= ~ I(1/dist^2)))</pre>
# Also syntactically correct since 'dist' is found in the data:
(fit <- fitme(time ~ dist + climb, data = hills, weights.form= ~ rep(2,length(dist))))
#### Programming with prior weights:
## Different ways of passing prior weights to fitme() from another function:
wrap_as_form <- function(weights.form) {</pre>
  fitme(time ~ dist + climb, data = hills, weights.form=weights.form)
wrap_as_pw <- function(prior.weights) {</pre>
  fitme(time ~ dist + climb, data = hills, prior.weights=prior.weights)
}
wrap_as_dots <- function(...) {</pre>
  fitme(time ~ dist + climb, data = hills,...)
}
```

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```
## Similarly for lm:
wrap_lm_as_dots <- function(...) {</pre>
 lm(time ~ dist + climb, data = hills, ...)
}
wrap_lm_as_arg <- function(weights) {</pre>
 lm(time ~ dist + climb, data = hills,weights=weights)
}
## Programming errors with stats::lm():
pw <- rep(1e-6,35) # or even NULL
(fit <- wrap_lm_as_arg(weights=pw)) # catches weights from global envir!</pre>
(fit <- lm(time ~ dist + climb, data = hills, weights=pw)) # idem!
(fit <- lm(time ~ dist + climb, data = hills,
           weights=hills$pw)) # fails silently - no $pw in 'hills'
(fit <- wrap_lm_as_dots(weights=hills$pw)) # idem!</pre>
(fit <- wrap_lm_as_arg(weights=hills$pw)) # idem!</pre>
## Safer spaMM results:
try(fit <- wrap_as_pw(prior.weights= pw)) # correctly catches problem</pre>
try(fit <- wrap_as_dots(prior.weights=hills$pw)) # correctly catches problem</pre>
(fit <- wrap_as_dots(prior.weights=1/dist^2)) # correct</pre>
(fit <- wrap_as_dots(prior.weights=quote(1/dist^2))) # correct</pre>
## But 'prior.weights' limitations:
try(fit <- wrap_as_pw(prior.weights= 1/hills$dist^2)) # fails (stop)</pre>
try(fit <- wrap_as_pw(prior.weights= 1/dist^2)) # fails (stop)</pre>
try(fit <- wrap_as_pw(prior.weights= quote(1/dist^2))) # fails (stop)</pre>
## Problems all solved by using 'weights.form':
try(fit <- wrap_as_form(weights.form= ~ pw)) # correctly catches problem</pre>
(fit <- wrap_as_form(weights.form= ~1/dist^2)) # correct</pre>
(fit <- wrap_as_form(weights.form= ~1/hills$dist^2)) # correct</pre>
(fit <- wrap_as_dots(weights.form= ~ 1/dist^2)) # correct</pre>
rm("pw")
```

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### **Description**

Loading these data loads three objects describing a mythical 'Gryphon' population used by Wilson et al. to illustrate mixed-effect modelling in quantitative genetics. These objects are a data frame Gryphon\_df containing the model variables, a genetic relatedness matrix Gryphon\_A, and another data frame Gryphon\_pedigree containing pedigree information (which can be used by some packages to reconstruct the relatedness matrix).

### Usage

```
data("Gryphon")
```

#### **Format**

Gryphon\_df is

```
'data.frame': 1084 obs. of 6 variables:

$ ID : int 1029 1299 ...: individual identifier

$ sex : Factor w/ 2 levels "1","2": sex, indeed

$ year : Factor w/ 34 levels "968","970", ...: birth year

$ mother: Factor w/ 429 levels "1","2",...: individual's mother identifier

$ BWT : num 10.77 9.3 ...: birth weight

$ TARSUS: num 24.8 22.5 12 ...: tarsus length
```

 ${\tt Gryphon\_A}\ is\ a\ genetic\ relatedness\ matrix, in\ sparse\ matrix\ format,\ for\ 1309\ individuals.$ 

Gryphon\_pedigree is

```
'data.frame': 1309 obs. of 3 variables:

$ ID : int 1306 1304 ...: individual identifier

$ Dam : int NA NA ...: individual's mother

$ Sire: int NA NA ...: individual's father
```

#### References

Wilson AJ, et al. (2010) An ecologist's guide to the animal model. Journal of Animal Ecology 79(1): 13-26. doi:10.1111/j.13652656.2009.01639.x

```
#### Bivariate-response model used as example in Wilson et al. (2010):
# joint modelling of birth weight (BWT) and tarsus length (TARSUS).

# The relatedness matrix is specified as a 'corrMatrix'. The random
# effect 'corrMatrix(0+mv(1,2)|ID)' then represents genetic effects
# correlated over traits and individuals (see help("composite-ranef")).
# The ...(0+...) syntax avoids contrasts being used in the design
# matrix of the random effects, as it would not does make much sense
# to represent TARSUS as a contrast to BWT.

# The relatedness matrix will be specified through its inverse,
# using as_precision(), so that spaMM does not have to find out and
```

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```
# inform the user that using the inverse is better (as is typically
# the case for relatedness matrices). But using as_precision() is
# not required. See help("algebra") for Details.
# The second random effect '(0+mv(1,2)|ID)' represents correlated
# environmental effects. Since measurements are not repeated within
# individuals, this effect also absorbs all residual variation. The
# residual variances 'phi' must then be fixed to some negligible values
# in order to avoid non-identifiability.
if (spaMM.getOption("example_maxtime")>7) {
 data("Gryphon")
 gry_prec <- as_precision(Gryphon_A)</pre>
 gry_GE <- fitmv(</pre>
    submodels=list(BWT \sim 1 + corrMatrix(0+mv(1,2)|ID)+(0+mv(1,2)|ID),
                  TARSUS ~ 1 + corrMatrix(0+mv(1,2)|ID)+(0+mv(1,2)|ID)),
    fixed=list(phi=c(1e-6,1e-6)),
    corrMatrix = gry_prec,
   data = Gryphon_df, method = "REML")
 # Estimates are practically identical to those reported for package
 # 'asreml' (https://www.vsni.co.uk/software/asreml-r)
 # according to Supplementary File 3 of Wilson et al., p.7:
 lambda_table <- summary(gry_GE, digits=5,verbose=FALSE)$lambda_table</pre>
 by_spaMM <- na.omit(unlist(lambda_table[,c("Var.","Corr.")]))[1:6]</pre>
 by_asreml <- c(3.368449,12.346304,3.849875,17.646017,0.381463,0.401968)
 by_spaMM/by_asreml-1 # relative differences ~ O(1e-4)
}
```

hatvalues.HLfit

Leverage extractor for HLfit objects

# **Description**

This gets "leverages" or "hat values" from an object. However, there is hidden complexity in what this may mean, so care must be used in selecting proper arguments for a given use (see Details). To get the full hat matrix, see get\_matrix(., which="hat\_matrix").

# Usage

```
## S3 method for class 'HLfit'
hatvalues(model, type = "projection", which = "resid", force=FALSE, ...)
```

### **Arguments**

model

An object of class HLfit, as returned by the fitting functions in spaMM.

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Character: "projection", "std", or more cryptic values not documented here.

See Details.

Which Character: "resid" for the traditional leverages of the observations, "ranef" for random-effect leverages, or "both" for both.

Force Boolean: to force recomputation of the leverages even if they are available in the object, for checking purposes.

For consistency with the generic.

#### **Details**

Leverages may have distinct meaning depending on context. The textbook version for linear models is that leverages  $(q_i)$  are the diagonal elements of a projection matrix ("hat matrix"), and that they may be used to standardize ("studentize") residuals as follows. If the residual variance  $\phi$  is known, then the variance of each fitted residual  $\hat{e}_i$  is  $\phi(1-q_i)$ . Standardized residuals, all with variance 1, are then  $\hat{e}_i/\surd(\phi(1-q_i))$ . This standardization of variance no longer holds exactly with estimated  $\phi$ , but if one uses here an unbiased (REML) estimator of  $\phi$ , the studentized residuals may still practically have a unit expected variance.

When a simple linear model is fitted by ML, the variance of the fitted residuals is less than  $\phi$ , but  $\hat{\phi}$  is downward biased so that residuals standardized only by  $\sqrt{(\phi)}$ , without any leverage correction, more closely have expected unit variance than if corrected by the previous leverages. The ML and REML computations can be seen as both using "standardizing" leverages, defined so that they are zero in the ML case and are equal to the "projection" leverages (the above ones, derived from a projection matrix) in the REML case.

These "standardizing" leverages can themselves been seen as special cases of those that appear in expressions for derivatives, with respect to the dispersion parameters, of the log-determinant of the information matrices considered in the Laplace approximation for marginal or restricted likelihood (Lee et al. 2006). This provides a basis to generalize the concept of standardizing leverages for ML and REML in mixed-effect models. In particular, in an ML fit, one considers leverages  $(q*_i)$  that are no longer the diagonal elements of the projection matrix for the mixed model [and, as hinted above, for a simple linear model the ML  $(q*_i)$  are zero]. The generalized standardizing leverages may include corrections for non-Gaussian response, for non-Gaussian random effects, and for taking into account the variation of the GLM weights in the logdet(info.mat) derivatives. Which corrections are included depend on the precise method used to fit the model (e.g., EQL vs PQL vs REML). Standardizing leverages are also defined for the random effects.

These distinctions suggest breaking the usual synonymy between "leverages" or "hat values": the term "hat values" better stands for the diagonal elements of a projection matrix, while "leverages" better stands for the standardizing values. hatvalues(.,type="std") returns the standardizing leverages. By contrast, hatvalues(.,type="projection") will always return hat values from the fitted projection matrix. Note that these values typically differ between ML and REML fit because the fitted projection matrix differs between them.

#### Value

A list with separate components resid (leverages of the observations) and ranef if which="both", and a vector otherwise.

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### References

Lee, Y., Nelder, J. A. and Pawitan, Y. (2006) Generalized linear models with random effects: unified analysis via h-likelihood. Chapman & Hall: London.

### **Examples**

**HLCor** 

Fits a (spatially) correlated mixed model, for given correlation parameters

### **Description**

A fitting function acting as a convenient interface for HLfit, constructing the correlation matrix of random effects from the arguments, then estimating fixed effects and dispersion parameters using HLfit. Various arguments are available to constrain the correlation structure, covStruct and distMatrix being the more general ones (for any number of random effects), and adjMatrix and corrMatrix being alternatives to covStruct for a single correlated random effect. uniqueGeo is deprecated.

### Usage

```
HLCor(formula, data, family = gaussian(), fixed=NULL, ranPars, distMatrix,
    adjMatrix, corrMatrix, covStruct=NULL,
    method = "REML", verbose = c(inner=FALSE),
    control.dist = list(), weights.form = NULL, ...)
```

### **Arguments**

formula

A predictor, i.e. a formula with attributes (see Predictor), or possibly simply a simple formula if an offset is not required.

fixed, ranPars

A list of given values for correlation parameters (some of which are mandatory), and possibly also dispersion parameters (optional, but passed to HLfit if present). ranPars is the old argument, maintained for back compatibility; fixed is the new argument, uniform across **spaMM** fitting functions. See ranPars for further information.

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data The data frame to be analyzed.

family A family object describing the distribution of the response variable. See HLfit

for further information.

distMatrix Either a distance matrix between geographic locations, forwarded to MaternCorr

or CauchyCorr. It overrides the (by default, Euclidean) distance matrix that would otherwise be deduced from the variables in a Matern(.) or Cauchy(.)

term;

**or** a list of such matrices. The list format is useful when there are several Matern/Cauchy terms, to avoid that all of them are affected by the same distMatrix.

NULL list elements may be necessary, e.g.

distMatrix=list("1"=NULL,"2"=<.>)) when a matrix is specified only for

the second random effect.

adjMatrix An single adjacency matrix, used if a random effect of the form

y ~ adjacency(1|<location index>) is present. See adjacency for further details. If adjacency matrices are needed for several random effects, use covStruct.

corrMatrix A matrix C used if a random effect term of the form corrMatrix(1|<stuff>)

is present. This allows to analyze non-spatial model by giving for example a matrix of genetic correlations. Each row corresponds to levels of a variable <stuff>. The covariance matrix of the random effects for each level is then  $\lambda \mathbf{C}$ , where as usual  $\lambda$  denotes a variance factor for the random effects (if  $\mathbf{C}$  is a correlation matrix, then  $\lambda$  is the variance, but other cases are possible). See corrMatrix for further details. If matrices are needed for several random

effects, use covStruct.

An interface for specifying correlation structures for different types of random

effect (corrMatrix or adjacency). See covStruct for details.

method Character: the fitting method to be used, such as "ML", "REML" or "PQL/L".

"REML" is the default. Other possible values of HLfit's method argument are

handled.

weights.form Specification of prior weights by a one-sided formula: use weights.form = ~

pw instead of prior.weights = pw. The effect will be the same except that such an argument, known to evaluate to an object of class "formula", is suitable to

enforce safe programming practices (see good-practice).

verbose A vector of booleans. inner controls various diagnostic (possibly messy) mes-

sages about the iterations. This should be distinguished from the TRACE element,

 $meaningful\ in\ {\tt fitme}\ or\ {\tt corr} {\tt HLfit}\ calls.$ 

control.dist A list of arguments that control the computation of the distance argument of the

correlation functions. Possible elements are

**rho.mapping** a set of indices controlling which elements of the rho scale vector scales which dimension(s) of the space in which (spatial) correlation matrices of random effects are computed. See same argument in make\_scaled\_dist

for details and examples.

**dist.method** method argument of proxy::dist function (by default, "Euclidean", but see make\_scaled\_dist for other distances such as spherical ones.)

Further parameters passed to HLfit or to mat\_sqrt.

. . .

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#### **Details**

For approximations of likelihood, see method. For the possible structures of random effects, see random-effects, but note that HLCor cannot adjust parameters of correlation models (with the exception of conditional autoregressive ones). Any such parameter must be specified by the ranPars argument. More generally, the correlation matrix for random effects can be specified by various combinations of formula terms and other arguments (see Examples):

**Basic Matérn model** Matern(1|<...>), using the spatial coordinates in <...>. This will construct a correlation matrix according to the Matérn correlation function (see MaternCorr);

**Basic Cauchy model** Cauchy(1|<...>), as for Matern (see CauchyCorr);

**Same models with given distance matrix** as provided by distMatrix (see Examples);

**Given correlation matrix** corrMatrix(1|<...>) with corrMatrix argument. See corrMatrix for further details.

**CAR model with given adjacency matrix** adjacency(1|<...>) with adjMatrix. See adjacency for further details;

**AR1 model** AR1(1 < ... >) See AR1 for further details.

#### Value

The return value of an HLfit call, with the following additional attributes:

```
HLCorcall the HLCor call info.uniqueGeo Unique geographic locations.
```

#### See Also

autoregressive for additional examples, MaternCorr, HLfit, and corrHLfit

HLfit

Fit mixed models with given correlation matrix

### **Description**

This function fits GL(M)Ms as well as some hierarchical generalized linear models (HGLM; Lee and Nelder 2001). It may be called on its own but is now better seen as a backend for the main fitting function fitme (or fitmv for multivariate-response models). This documentation completes the documentation of the latter functions with respect to some arguments they pass to HLfit and with respect to the structure of the objects they return.

On its own, HLfit fits both fixed effects parameters, and dispersion parameters i.e. the variance of the random effects (full covariance for random-coefficient models), and the variance of the residual error. The linear predictor is of the standard form offset+ X beta + Z b, where X is the design matrix of fixed effects and Z is a design matrix of random effects (typically an incidence matrix with 0s and 1s, but not necessarily). Models are fitted by an iterative algorithm alternating estimation of fixed effects and of dispersion parameters. The residual dispersion may follow a "structured-dispersion model" modeling heteroscedasticity. Estimation of the latter parameters is performed by a form of fit of debiased residuals, which allows fitting a structured-dispersion model (Smyth et al. 2001). However, evaluation of the debiased residuals can be slow in particular for large datasets. For models without structured dispersion, it is then worth using the fitme function. Ths function (as well as corrHLfit) can optimize the likelihood of HLfit fits for different given values of the dispersion parameters ("outer optimization"), thereby avoiding the need to estimate debiased residuals.

# Usage

```
HLfit(formula, data, family = gaussian(), rand.family = gaussian(),
    resid.model = ~1, REMLformula = NULL, verbose = c(inner = FALSE),
    HLmethod = "HL(1,1)", method="REML", control.HLfit = list(),
    control.glm = list(), init.HLfit = list(), fixed=list(), ranFix,
    etaFix = list(), prior.weights = NULL, weights.form = NULL,
    processed = NULL)
## see 'rand.family' argument for inverse.Gamma
```

# Arguments

formula	A formula; or a predictor, i.e. a formula with attributes created by Predictor, if design matrices for random effects have to be provided. See Details in spaMM for allowed terms in the formula (except spatial ones).
data	A data frame containing the variables named in the model formula.
family	A family object describing the distribution of the response variable. See Details in spaMM for handled families.
rand.family	A family object describing the distribution of the random effect, or a list of family objects for different random effects (see Examples). Possible options are gaussian(), Gamma(log), Gamma(identity) (see Details), Beta(logit), inverse.Gamma(-1/mu), and inverse.Gamma(log). For discussion of these

alternatives see Lee and Nelder 2001 or Lee et al. 2006, p. 178-. Here the family gives the distribution of a random effect u and the link gives v as function of u (see Details). If there are several random effects and only one family is given, this family holds for all random effects.

resid.model

Used to specify a model for the dispersion parameter of the mean-response family. See the resid.model documentation, and the more specific phi-resid.model one for the phi parameter of gaussian and Gamma response families.

REMLformula

A model formula that controls the estimation of dispersion parameters and the computation of restricted likelihood (p\_bv), where the conditioning inherent in REML is defined by a model different from the predictor formula. A simple example (useless in practice) of its effect is to replicate an ML fit by specifying method="REML" and an REMLformula with no fixed effect. The latter implies that no conditioning is performed and that p\_bv equals the marginal likelihood (or its approximation), p\_v. One of the examples in update.HLfit shows how REMLformula can be useful, but otherwise this argument may never be needed for standard REML or ML fits. For non-standard likelihood ratio tests using REMLformula, see fixedLRT.

verbose

A vector of booleans or integers. The inner element controls various diagnostic messages (possibly messy) about the iterations. This should be distinguished from the TRACE element, meaningful in fitme or corrHLfit calls, and much more useful. The phifit element controls messages about the progress of phi-resid.model fits (see the latter documentation).

method

Character: the fitting method. allowed values include "REML", "ML", "EQL-" and "EQL+" for all models, and "PQL" (="REPQL") and "PQL/L" for GLMMs only. method=c(<"ML" or "REML">, "exp") can be distinctly useful for slow fits of models with Gamma(log) response family. See (see method) for details, and further possible values for those curious to experiment. The default is REML (standard REML for LMMs, an extended definition for other models). REML can be viewed as a form of conditional inference, and non-standard conditionings can be called by using a non-standard REML formula.

**HLmethod** 

Same as method. It is useless to specify HLmethod when method is specified. The default value "HL(1,1)" means the same as method="REML", but more accurately relates to definitions of approximations of likelihood in the h-likelihood literature.

control.HLfit

A list of parameters controlling the fitting algorithms, which should mostly be ignored in routine use. See control.HLfit for possible controls.

control.glm

List of parameters controlling calls to glm-"like" fits, passed to glm.control; e.g.

control.glm=list(maxit=100). See glm.control for further details. glm-"like" fits may be performed as part of mixed-effect model fitting procedures, in particular to provide initial values (possibly using llm.fit for non-GLM families), and for "inner" estimation of dispersion parameters.

init.HLfit

A list of initial values for the iterative algorithm, with possible elements of the list are fixef for fixed effect estimates (beta), v\_h for random effects vector  ${\bf v}$  in the linear predictor, lambda for the parameter determining the variance of random effects u as drawn from the rand.family distribution, and phi for the residual variance. However, this argument can be ignored in routine use.

fixed, ranFix A list of fixed values of random effect parameters. ranFix is the old argument,

maintained for back compatibility; fixed is the new argument, uniform across

**spaMM** fitting functions. See ranFix for further information.

etaFix A list of given values of the coefficients of the linear predictor. See etaFix for

further information.

prior.weights An optional vector of prior weights as in glm. This fits the data to a probability

model with residual variance parameter given as phi/prior.weights instead of the canonical parameter phi of the response family, and all further outputs

are defined to be consistent with this (see section IV in Details).

weights.form Specification of prior weights by a one-sided formula: use weights.form = ~

pw instead of prior.weights = pw. The effect will be the same except that such an argument, known to evaluate to an object of class "formula", is suitable to

enforce safe programming practices (see good-practice).

processed A list of preprocessed arguments, for programming purposes only.

#### **Details**

I. Approximations of likelihood: see method.

**II. Possible structure of Random effects:** see random-effects, but note that HLfit does not fit models with autocorrelated random effects.

III. The standard errors reported may sometimes be misleading. For each set of parameters among  $\beta$ ,  $\lambda$ , and  $\phi$  parameters these are computed assuming that the other parameters are known without error. This is why they are labelled Cond. SE (conditional standard error). This is most uninformative in the unusual case where  $\lambda$  and  $\phi$  are not separately estimable parameters. Further, the SEs for  $\lambda$  and  $\phi$  are rough approximations as discussed in particular by Smyth et al. (2001;  $V_1$  method).

**IV. prior weights**. This controls the likelihood analysis of heteroscedastic models. In particular, changing the weights by a constant factor f should, and will, yield a fit with unchanged likelihood and (Intercept) estimates of phi also increased by f (except if a non-trivial resid. formula with log link is used). This is consistent with what glm does, but other packages may not follow this logic (whatever their documentation may say: check by yourself by changing the weights by a constant factor). Further, post-fit functiosn (in particular those extracting various forms of residuals) may be inconsistent in their handling of prior weights.

#### Value

An object of class HLfit, which is a list with many elements, not all of which are documented.

Various extractor functions are available (see extractors, vcov, get\_fittedPars, get\_matrix, and so on). They should be used as far as possible as they should be backward-compatible from version 2.0.0 onwards, while the structure of the return object may still evolve. The following information may be useful for extracting further elements of the object.

Elements include **descriptors of the fit**:

eta Fitted values on the linear scale (including the predicted random effects). predict(.,type="link") can be used as a formal extractor;

fv Fitted values ( $\mu = \text{sinverse-link}(\eta)$ ) of the response variable. fitted(.) or

predict(.) can be used as formal extractors;

fixef The fixed effects coefficients,  $\beta$  (returned by the fixef function);

 $v_h$  The random effects on the linear scale,  $v_h$  with attribute the random effects  $u_h$ 

(returned by ranef(\*, type="uncorrelated");

phi The residual variance  $\phi$ . See residVar for one extractor;

phi.object A possibly more complex object describing  $\phi$  (see residVar again);

lambda The random-effect (u) variance(s)  $\lambda$  in compact form;

lambda.object A possibly more complex object describing  $\lambda$  (see get\_ranPars(.,which="lambda"))

and VarCorr extractors);

ranef\_info environment where information about the structure of random effects is stored

(see Corr);

corrPars Agglomerates information on correlation parameters, either fixed, or estimated

((see get\_ranPars(.,which="corrPars")));

APHLs A list whose elements are various likelihood components, including conditional

likelihood, h-likelihood, and the Laplace approximations: the (approximate) marginal **likelihood**  $p_v$  and the (approximate) **restricted likelihood**  $p_v$  (the latter two available through the logLik function). See the extractor function  $get_any_IC$  for information criteria ("AIC") and effective degrees of freedom;

The covariance matrix of  $\beta$  estimates is not included as such, but can be extracted by vcov.

**Information about the input** is contained in output elements named as arguments of the fitting function calls (data, family, resid.family, ranFix, prior.weights), with the following notable exceptions or modifications:

predictor The formula, possibly reformatted (returned by the formula extractor);

resid.predictor

Analogous to predictor, for the residual variance (see residVar(., which="formula"));

rand.families corresponding to the rand.family input;

### Further miscellaneous diagnostics and descriptors of model structure:

X.pv The design matrix for fixed effects (returned by the model.matrix extractor);

ZAlist, strucList

Two lists of matrices, respectively the design matrices "Z", and the "L" matrices, for the different random-effect terms. The extractor get\_ZALMatrix can be used

to reconstruct a single "ZL" matrix for all terms.

BinomialDen (binomial data only) the binomial denominators;

y the response vector; for binomial data, the frequency response.

models Additional information on model structure for  $\eta$ ,  $\lambda$  and  $\phi$ ;

HL A set of indices that characterize the approximations used for likelihood;

leve\_phi, lev\_lambda

Leverages (see hatvalues extractor);

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dfs list (possibly structured): some information about degrees of freedom for differ-

ent components of the model. But its details may be difficult to interpret and the

DoF extractor should be used;

how A list containing the information properly extracted by the how function;

warnings A list of warnings for events that may have occurred during the fit.

Finally, the object includes programming tools: call, spaMM.version, fit\_time and an environment envir that may contain whatever may be needed in some post-fit operations.

#### References

Lee, Y., Nelder, J. A. (2001) Hierarchical generalised linear models: A synthesis of generalised linear models, random-effect models and structured dispersions. Biometrika 88, 987-1006.

Lee, Y., Nelder, J. A. and Pawitan, Y. (2006). Generalized linear models with random effects: unified analysis via h-likelihood. Chapman & Hall: London.

Smyth GK, Huele AF, Verbyla AP (2001). Exact and approximate REML for heteroscedastic regression. Statistical Modelling 1, 161-175.

#### See Also

HLCor for estimation with given spatial correlation parameters; corrHLfit for joint estimation with spatial correlation parameters; fitme as an alternative to all these functions.

# **Examples**

how

Extract information about how an object was obtained

#### **Description**

how is defined as a generic with currently only one non-default method, for objects of class HLfit. This method provide information about how such a fit was obtained.

# Usage

```
how(object, ...)
## S3 method for class 'HLfit'
how(object, devel=FALSE, verbose=TRUE, format=print, ...)
## S3 method for class 'HLfitlist'
how(object, devel=FALSE, verbose=TRUE, format=print, ...)
```

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### Arguments

object	Any R object.
devel	Boolean; Whether to provide additional cryptic information. For development purposes, not further documented.
verbose	Boolean; Whether to print information about the input object.
format	wrapper for printing format. E.g., $cat(crayon::yellow(s),"\n")$ could be used instead of the default.
	Other arguments that may be needed by some method.

#### Value

A list, returned invisibly, whose elements are not further described here, some being slightly cryptic or subject to future changes However, how(.)\$fit\_time is a clean way of getting the fit time. If verbose is TRUE, the function prints a message presenting some of these elements.

# **Examples**

```
foo <- HLfit(y~x, data=data.frame(x=runif(3), y=runif(3)), method="ML", ranFix=list(phi=1))
how(foo)</pre>
```

inits Controlling optimization strategy through initial values	
--	--

## Description

Several parameters (notably the dispersion parameters: the variance of random effects and the residual variance parameter, if any) can be estimated either by iterative algorithms, or by generic optimization methods. The development of the fitme function aims to provide full control of the selection of algorithms. For example, if two random effects are fitted, then

init=list(lambda=c(NA,NaN)) enforces generic optimization for the first variance and iterative algorithms for the second.

init=list(lambda=c(0.1,NaN)) has the same effect and additionally provides control of the initial value for optimization (whereas init.HLfit=list(lambda=c(NA,0.1)) will provide control of the initial value for iterations).

How to know which algorithm has been selected for each parameter? fitme(., verbose=c(TRACE=TRUE)) shows successive values of the variables estimated by optimization (See Examples; if no value appears, then all are estimated by iterative methods). The first lines of the summary of a fit object should tell which variances are estimated by the "outer" method.

corrHLfit, which uses inner optimization by default, can be forced to perform outer optimization. Its control is more limited, as NAs and NaNs are not allowed. Instead, only numeric values as in init=list(lambda=0.1) are allowed.

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### **Examples**

```
## Not run:
air <- data.frame(passengers = as.numeric(AirPassengers),</pre>
                  year_z = scale(rep(1949:1960, each = 12)),
                  month = factor(rep(1:12, 12)))
air$time <- 1:nrow(air)
# Use verbose to find that lambda is estimated by optimization
fitme(passengers ~ month * year_z + AR1(1|time), data = air,
      verbose=c(TRACE=TRUE))
# Use init to enforce iterative algorithm for lambda estimation:
fitme(passengers ~ month * year_z + AR1(1|time), data = air,
      verbose=c(TRACE=TRUE), init=list(lambda=NaN))
# (but then it may be better to enforce it also for phi: init=list(lambda=NaN, phi=NaN))
# Use init to enforce generic optimization for lambda estimation,
   and control initial value:
fitme(passengers ~ month * year_z + AR1(1|time), data = air,
      verbose=c(TRACE=TRUE), init=list(lambda=0.1))
# See help("multinomial") for more examples of control by initial values.
## End(Not run)
```

inverse.Gamma

Distribution families for Gamma and inverse Gamma-distributed random effects

# **Description**

For dispersion parameter  $\lambda$ , Gamma means that random effects are distributed as u Gamma(shape= $1/\lambda$ ,scale= $\lambda$ ), so u has mean 1 and variance  $\lambda$ . Both the log (v = log(u)) and identity (v = u) links are possible, though in the latter case the variance of u is constrained below 1 (otherwise Laplace approximations fail)

The two-parameter inverse Gamma distribution is the distribution of the reciprocal of a variable distributed according to the Gamma distribution Gamma with the same shape and scale parameters. inverse Gamma implements the one-parameter inverse Gamma family with shape=1+1/ $\lambda$  and rate=1/ $\lambda$ ) (rate=1/scale). It is used to model the distribution of random effects. Its mean=1; and its variance = $\lambda/(1-\lambda)$ ) if  $\lambda<1$ , otherwise infinite. The default link is "-1/mu", in which case v=-1/u is "-Gamma"-distributed with the same shape and rate, hence with mean  $-(\lambda+1)$  and variance  $\lambda(\lambda+1)$ , which is a different one-parameter Gamma family than the above-described Gamma. The other possible link is v=log(u) in which case

```
v - \log(X \operatorname{Gamma}(1 + 1/\lambda, 1/\lambda)), with mean -(\log(1/\lambda) + \operatorname{digamma}(1 + 1/\lambda)) and variance trigamma(1 + 1/\lambda).
```

#### Usage

```
inverse.Gamma(link = "-1/mu")
# Gamma(link = "inverse") using stats::Gamma
```

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### Arguments

link For Gamma, allowed links are log and identity (the default link from Gamma,

"inverse", cannot be used for the random effect specification). For inverse . Gamma,

allowed links are "-1/mu" (default) and log.

#### **Examples**

# see help("HLfit") for fits using the inverse. Gamma distribution.

is\_separated

Checking for (quasi-)separation in binomial-response model.

### **Description**

Separation occurs in binomial response models when a combination of the predictor variables perfectly predict a level of the response. In such a case the estimates of the coefficients for these variables diverge to (+/-)infinity, and the numerical algorithms typically fail. To anticipate such a problem, the fitting functions in spaMM try to check for separation by default. The check may take much time, and is skipped if the "problem size" exceeds a threshold defined by spaMM.options(separation\_max=<.>), in which case a message will tell users by how much they should increase separation\_max to force the check (its exact meaning and default value are subject to changes without notice but the default value aims to correspond to a separation check time of the order of 1s on the author's computer).

is\_separated is a convenient interface to procedures from the ROI package, allowing them to be called explicitly by the user to check bootstrap samples (see Example in anova). is\_separated.formula is a variant (not yet a formal S3 method) that performs the same check, but using arguments similar to those of fitme(., family=binomial()).

### Usage

### **Arguments**

x Design matrix for fixed effects.y Numeric response vector

formula A model formula

... data and possibly other arguments of a fitme call. family is ignored if present. separation\_max numeric: non-default value allow for easier local control of this spaMM option.

solver character: name of linear programming solver used to assess separation; passed

to ROI\_solve's solver argument. One can select another solver if the corre-

sponding ROI plugin is installed.

verbose Whether to print some messages (e.g., pointing model terms that cause separa-

tion) or not.

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#### Value

Returns a boolean; TRUE means there is (quasi-)separation. Screen output may give further information, such as pointing model terms that cause separation.

#### References

The method accessible by solver="glpk" implements algorithms described by

Konis, K. 2007. Linear Programming Algorithms for Detecting Separated Data in Binary Logistic Regression Models. DPhil Thesis, Univ. Oxford. https://ora.ox.ac.uk/objects/uuid:8f9ee0d0-d78e-4101-9ab4-f9cbceed2a2a.

#### See Also

See also the 'safeBinaryRegression' and 'detectseparation' package.

### **Examples**

```
set.seed(123)
d <- data.frame(success = rbinom(10, size = 1, prob = 0.9), x = 1:10)
is_separated.formula(formula= success~x, data=d) # FALSE
is_separated.formula(formula= success~I(success^2), data=d) # TRUE</pre>
```

Leuca

Leucadendron data

# **Description**

A data set from Tonnabel et al. (2021) to be fitted by models with sex-specific spatial random effects. Leucadrendron rubrum is a dioecious shrub from South Africa. Various phenotypes were recorded on individuals from a small patch of habitat.

#### Usage

```
data("Leuca")
```

## Format

Leuca is

```
'data.frame': 156 obs. of 12 variables:

$ name : Factor w/ 156 levels "f_101", "f_102",..: 1 2 3 4 5 6 7 8 9 10 ...

$ sex : Factor w/ 2 levels "f", "m": 1 1 1 1 1 1 1 1 1 1 1 ...

$ area : num    0.857    0.9    0.827    0.654    0.733 ...

$ diam : int    60    30    180    50    70    80    130    90    27    59 ...

$ fec : num    0.013    0.0137    5.1171    0.2905    1.042 ...

$ fec_div: num    0.0128    0.0135    5.037    0.2859    1.0257 ...

$ x : num    42 41 62.5    58.5    42.5    33.5    24    26.5    25    41 ...
```

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```
$ y : num 23 46 58 63 51 51 55.5 55.5 58.5 63 ...
$ diamZ : num -0.713 -1.479 2.352 -0.968 -0.457 ...
$ areaZ : num 0.72 0.92 0.586 -0.2 0.158 ...
$ male : logi FALSE FA
```

### **Source**

Tonnabel, J., Klein, E.K., Ronce, O., Oddou-Muratorio, S., Rousset, F., Olivieri, I., Courtiol, A. and Mignot, A. (2021), Sex-specific spatial variation in fitness in the highly dimorphic Leucadendron rubrum. Mol Ecol, 30: 1721-1735. doi:10.1111/mec.15833

#### See Also

MaternCorr and composite-ranef for examples using these data.

## **Examples**

data(Leuca)

lev2bool

Conversion of factor to 0/1 variable

### **Description**

It may be straightforward to add columns of indicator variables for each level of a factor to the data, by

< data > < - cbind(< data > , model.matrix( ~ < factor > - 1, data = < data >)). Alternatively, indicator variables can be created on the fly for given levels, using the lev2bool function.

# Usage

```
lev2bool(fac, lev)
```

### **Arguments**

fac An object coercible to factor.

lev The level of fac to be converted to 1.

# Value

A one-column matrix.

#### See Also

Example in GxE for alternative to using lev2bool in specification of random effects with heteroscedasticity, useful when the latter is controlled by a factor with many levels.

Ilm.fit

### **Examples**

```
## Elementary bivariate-response model
# Data preparation
#
fam <- rep(c(1,2),rep(6,2)) # define two biological 'families'
ID <- gl(6,2) # define 6 'individuals'</pre>
resp <- as.factor(rep(c("x","y"),6)) # distinguishes two responses per individual
set.seed(123)
toymv <- data.frame(</pre>
 fam = factor(fam), ID = ID, resp = resp,
 y = 1 + (resp=="x") + rnorm(4)[2*(resp=="x")+fam] + rnorm(12)[6*(resp=="x")+as.integer(ID)]
toymv <- cbind(toymv, model.matrix( ~ resp - 1, data = toymv))</pre>
# fit response-specific variances of random effect and residuals:
(fitme(y ~ resp+ (0+respx|fam)+ (0+respy|fam),
        resid.model = ~ 0+resp ,data=toymv))
# Same result by different syntaxes:
# * by the lev2bool() specifier:
(fitme(y \sim resp+ (0+lev2bool(resp, "x")|fam)+ (0+lev2bool(resp, "y")|fam),
        resid.model = ~ 0+resp ,data=toymv))
# * or by random-coefficient model using 'resp' factor:
(fitme(y ~ resp+ (0+resp|fam), resid.model = ~ 0+resp ,data=toymv,
       fixed=list(ranCoefs=list("1"=c(NA,0,NA)))))
#
# For factors with more levels, the following function may be useful to specify
# through partially fixed ranCoefs that covariances are fixed to zero:
ranCoefs_for_diag <- function(nlevels) {</pre>
 vec <- rep(0,nlevels*(nlevels+1L)/2L)</pre>
 vec[cumsum(c(1L,rev(seq(nlevels-1L)+1L)))] <- NA</pre>
}
# see application in help("GxE").
# * or by the dummy() specifier from lme4:
# (fitme(y ~ resp+ (0+dummy(resp,"x")|fam)+ (0+dummy(resp,"y")|fam),
         resid.model = ~ 0+resp ,data=toymv))
```

llm.fit

*Link-linear regression models (LLMs)* 

### **Description**

Some "family" objects in **spaMM** describe models with non-GLM response families, such as the negbin1 or beta\_resp families already widely considered in previous works and other packages.

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These models are characterized by a linear predictor, a link function, and a distribution for residual variation that does not belong to the exponential family from which GLMs are defined.

These family objects are conceived for use with **spaMM**'s fitting functions. They cannot generally be used as argument to the glm function, except when this function is highjacked by use of the method="llm.fit" argument, where llm stands for Link-Linear (as in "log-linear", say) regression Model.

Mixed-effect models fitted by such methods cannot use expected-Hessian approximations, in contrast to GLM response families. negbin2 is a family object for a GLM response family (strictly speaking, only for fixed shape and untruncated version) but implemented as an LL-family, in particular using only the observed Hessian matrix.

### Usage

```
# glm(..., method="llm.fit")
## See also 'beta_resp', 'negbin1', 'betabin', and possibly later additions.
```

#### **Details**

These family objects are lists, formally of class c("LLF", "family"). Compared to a family object, they have additional elements, not documented here.

As stats:: GLM family objects do, they provide deviance residuals through the dev.resids member function. There are various definitions of deviance residuals for non-GLM families in the literature. Here they are defined as "2\*(saturated\_logLik - logLik)", where the likelihood for the saturated model is the likelihood maximized wrt to the mean parameter  $\mu$  for each observation y independently. The maximizing  $\mu$  is not equal to the observation, in contrast to the standard result for GLMs.

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```
(var_prec <- fitme(y ~1, family=beta_resp(), data= beta_dat))
# Highjacking glm():
fitted_prec <- residVar(var_prec,which="fam_parm")
glm(y ~1, family=beta_resp(prec=fitted_prec), data= beta_dat, method="llm.fit")</pre>
```

Loaloa

Loa loa prevalence in North Cameroon, 1991-2001

## **Description**

This data set describes prevalence of infection by the nematode *Loa loa* in North Cameroon, 1991-2001. This is a superset of the data discussed by Diggle and Ribeiro (2007) and Diggle et al. (2007). The study investigated the relationship between altitude, vegetation indices, and prevalence of the parasite.

### Usage

```
data("Loaloa")
```

#### **Format**

The data frame includes 197 observations on the following variables:

latitude latitude, in degrees.

longitude longitude, in degrees.

**ntot** sample size per location

npos number of infected individuals per location

maxNDVI maximum normalised-difference vegetation index (NDVI) from repeated satellite scans

seNDVI standard error of NDVI

elev1 altitude, in m.

**elev2,elev3,elev4** Additional altitude variables derived from the previous one, provided for convenience: respectively, positive values of altitude-650, positive values of altitude-1000, and positive values of altitude-1300

maxNDVI1 a copy of maxNDVI modified as maxNDVI1[maxNDVI1>0.8] <- 0.8

## Source

The data were last retrieved on March 1, 2013 from P.J. Ribeiro's web resources at www.leg.ufpr.br/doku.php/pessoais:paulojus:mbgbook:datasets. A current (2022-06-18) source is https://www.lancaster.ac.uk/staff/diggle/moredata/Loaloa.txt).

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#### References

Diggle, P., and Ribeiro, P. 2007. Model-based geostatistics, Springer series in statistics, Springer, New York.

Diggle, P. J., Thomson, M. C., Christensen, O. F., Rowlingson, B., Obsomer, V., Gardon, J., Wanji, S., Takougang, I., Enyong, P., Kamgno, J., Remme, J. H., Boussinesq, M., and Molyneux, D. H. 2007. Spatial modelling and the prediction of Loa loa risk: decision making under uncertainty, Ann. Trop. Med. Parasitol. 101, 499-509.

```
data("Loaloa")
if (spaMM.getOption("example_maxtime")>5) {
  fitme(cbind(npos,ntot-npos)~1 +Matern(1|longitude+latitude),
        data=Loaloa, family=binomial())
}
### Variations on the model fit by Diggle et al.
      on a subset of the Loaloa data
### In each case this shows the slight differences in syntax,
###
      and the difference in 'typical' computation times,
      when fit using corrHLfit() or fitme().
if (spaMM.getOption("example_maxtime")>4) {
 corrHLfit(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI
                   +Matern(1|longitude+latitude), method="HL(0,1)",
                 data=Loaloa,family=binomial(),ranFix=list(nu=0.5))
}
if (spaMM.getOption("example_maxtime")>1.6) {
 fitme(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI
                   +Matern(1|longitude+latitude), method="HL(0,1)",
                 data=Loaloa, family=binomial(), fixed=list(nu=0.5))
}
if (spaMM.getOption("example_maxtime")>5.8) {
 corrHLfit(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI
            +Matern(1|longitude+latitude),
              data=Loaloa,family=binomial(),ranFix=list(nu=0.5))
}
if (spaMM.getOption("example_maxtime")>2.5) {
  fitme(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI
            +Matern(1|longitude+latitude),
              data=Loaloa,family=binomial(),fixed=list(nu=0.5),method="REML")
}
## Diggle and Ribeiro (2007) assumed (in this package notation) Nugget=2/7:
if (spaMM.getOption("example_maxtime")>7) {
 corrHLfit(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI
           +Matern(1|longitude+latitude),
             data=Loaloa,family=binomial(),ranFix=list(nu=0.5,Nugget=2/7))
if (spaMM.getOption("example_maxtime")>1.3) {
```

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```
fitme(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI
           +Matern(1|longitude+latitude), method="REML",
             data=Loaloa,family=binomial(),fixed=list(nu=0.5,Nugget=2/7))
}
## with nugget estimation:
if (spaMM.getOption("example_maxtime")>17) {
 corrHLfit(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI
           +Matern(1|longitude+latitude),
             data=Loaloa,family=binomial(),
             init.corrHLfit=list(Nugget=0.1),ranFix=list(nu=0.5))
}
if (spaMM.getOption("example_maxtime")>5.5) {
  fitme(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI
           +Matern(1|longitude+latitude),
             data=Loaloa,family=binomial(),method="REML",
             init=list(Nugget=0.1),fixed=list(nu=0.5))
}
```

LRT

ANOVA tables, and likelihood ratio tests of fixed and random effects.

### **Description**

The anova method for fit objects from **spaMM** has two uses: if a single fit object is provided, ANOVA tables may be returned, with specific procedures for univariate-response LMs, GLMs and LMMs (see Details). Alternatively, if a second fit object is provided (object2 argument), anova performs as an alias for LRT. The LRT function here differs from fixedLRT by its arguments (model fits for LRT, but all arguments required to fit the models for fixedLRT), and by the format of its return value.

LRT performs a likelihood ratio (LR) test between two model fits, the "full" and the "null" model fits. It determines which model is the more complete one by comparing model components including the fixed-effect, random-effect, residual-dispersion model specifications, and response families (offsets are ignored). Then, a standard test based on the asymptotic chi-square distribution is performed. In addition, parametric bootstrap p-values can be computed, either using the *raw bootstrap* distribution of the likelihood ratio, or a bootstrap estimate of the Bartlett correction of the LR statistic.

These different tests perform diffferently depending on the differences between the two models:

- \* If the models differ only by their fixed effects, the asymptotic LRT may be anticonservative, but the Bartlett-corrected one is generally well-calibrated.
- \* If the two models differ by their random effects, tests based on the chi-square distribution (including their Bartlett-corrected version) may be poorly behaved, as such tests assume unbounded parameters, as contrasted to, e.g., necessarily positive variances.

In such cases the raw boostrap test may be the only reliable test. The procedure aims to detect and report such issues, but may not report all problems: users remain responsible for applying the tests in valid conditions (see **Caveats** in Details section). In simple cases (such as comparing a

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fixed-effect to a mixed-effect model with the same fixed-effect term), the chi-square tests may not be reported. In other cases (see Examples) they may otherwise be reported, with a warning when the procedure detects some cases of estimates at the boundary for the full model, or detects cases where the LR statistic of bootstrap replicates is often zero (also suggesting that estimates are at the boundary in such replicates).

- \* If the fits differ by the fixed effects terms of their residual-dispersion models (but not by any random effect specification), tests based on the chi-square distribution are reported. A bootstrap can be performed as in other cases.
- \* Tests for some cases of nested response families (e.g., the Poisson versus its extensions) are tentatively allowed.
- \* In some cases the full and the null models cannot be identified and the basic LRT based on the chi-square distribution will not be returned, but a bootstrap test may still be performed.
- \* The case where residual-dispersion models of either fit include random effects is problematic as, for such fits, the fitting procedure does not maximize the reported likelihood. The basic LRT is not returned when the two fits differ by their random effects, but is still performed otherwise (see Examples); and a bootstrap test may still be performed in both cases.

### Usage

```
## S3 method for class 'HLfit'
anova(object, object2, type = "2", method="", ...)
#
LRT(object, object2, boot.repl = 0L, resp_testfn = NULL,
    simuland = eval_replicate,
    # many further arguments can be passed to spaMM_boot via the '...'
    # These include arguments for parallel computations, such as
    # nb_cores, fit_env,
    # as well as other named arguments and spaMM_boot's own '...'
    ...)
```

Fit abject naturally a grown fitting function

### **Arguments**

ab = a a +

models.

object	Fit object returned by a <b>spaMM</b> fitting function.
object2	Optional second model fit to be compared to the first (their order does not matter, except in non-standard cases where the second model is taken as teh null one and a message is issued).
type	ANOVA type for LMMs, as interpreted by <b>lmerTest</b> . Note that the default (single-term deletion ANOVA) differs from that of <b>lmerTest</b> .
boot.repl	the number of bootstrap replicates.
resp_testfn	See argument resp_testfn of spaMM_boot.
simuland	a function, passed to spaMM_boot. See argument eval_replicate for default value and requirements.
method	Only non-default value is "t.Chisq" which forces evaluation of a table of chisquared tests for each fixed-effect term, using the classical "Wald" test (see Details). Further methods are available through the for specific classes of

Further arguments, passed to spaMM\_boot (e.g., for parallelization) in the case of LRTs. For ANOVA tables, arguments of functions anova.lm anova.glm, and as\_LMLT, respectively for LMs, GLMs and LMMs, may be handled (e.g. the test argument for anova.glm).

#### **Details**

- \* The **ANOVA-table** functionality has been included here mainly to provide access to F tests (including, for LMMs, the "Satterthwaite method" as developed by Fai and Cornelius, 1996), using pre-existing procedures as template or backend for expediency and familiarity:
  - 1. ANOVA tables for LMs and GLMs have been conceived to replicate the functionality, output format and details of base R anova, and therefore replicate some of their limitations, e.g., they only perform sequential analysis ("type 1") in the same way as anova.lm and anova.glm. However, a difference occurs for Gamma GLMs, because the dispersion estimates for Gamma GLMs differ between stats::glm and spaMM fits (see Details in method). Therefore, F tests and Mallows' Cp differ too; results from spaMM REML fits being closer than ML fits to those from glm() fits;
  - 2. **For LMMs**, ANOVA tables are provided by interfacing lmerTest::anova (with non-default type). This procedure should handle all types of LMMs that can be fitted by **spaMM**; yet, the displayed information should be inspected to check that some fitted random-effect parameters are not ignored when computing information for the Satterthwaite method.
  - 3. For fitted models that do not lay within previous categories, such as GLMMs, models with a residual-dispersion submodel, and multivariate-response models, a table of tests for single-term deletions using the classical "Wald" chi-squared test based on coefficient values and their conditional standard error estimates will be returned. LRTs (moreover, with bootstrap correction) are more reliable than such tests and, as calling them requires a second model to be explicitly specified, they may also help users thinking about the hypothesis they are testing.
- \* Bootstrap LRTs: A raw bootstrap p-value can be computed from the simulated distribution as (1+sum(t>=t0))/(N+1) where t0 is the original likelihood ratio, t the vector of bootstrap replicates and t its length. See Davison & Hinkley (1997, p. 141) for discussion of the adjustments in this formula. However, a computationally more economical use of the bootstrap is to provide a Bartlett correction for the likelihood ratio test in small samples. According to this correction, the mean value t of the likelihood ratio statistic under the null hypothesis is computed (here estimated by a parametric bootstrap) and the original LR statistic is multiplied by t0 where t1 is the number of degrees of freedom of the test.

When models differ by their random-effect specifications, distinguishing the full from the null model is not easy. In particular, equivalent models can be specified by diverse syntaxes, so a simple textual comparison of the random-effect terms may not be enough, and model specifications that hinder such a comparison should be avoided. When differences in random effects are tested, the null distribution of the LR may include a probability mass in 1: the discussion in Details of get\_RLRsim\_args applies.

\* Caveats: (1) An evaluated log-likelihood ratio can be slightly negative, e.g. when a fixed-effect model is compared to a mixed one, or a spatial random effect to a block effect, if parameters of the more complete model are estimated within bounds (e.g., variance>1e-06, or Matern smoothness>0.005) designed to avoid numerical singularities, while the less complete model corresponds

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to a boundary case (e.g., variance=0, or smoothness=0). The bootstrap procedure tries to identify these cases and then corrects slightly negative logL ratios to 0. (2) The Bartlett correction is applicable when the true distribution of the LRT departs smoothly from the chi-square distribution, but not in cases where it has a probability mass in zero (at typically occurs in the same boundary cases).

#### Value

LRT returns an object of class fixedLRT, actually a list with typical elements (depending on the options)

fullfit the HLfit object for the full model; nullfit the HLfit object for the null model;

basicLRT A data frame including values of the likelihood ratio chi2 statistic, its degrees of

freedom, and the p-value;

and, if a bootstrap was performed:

rawBootLRT A data frame including values of the likelihood ratio chi2 statistic, its degrees of

freedom, and the raw bootstrap p-value;

BartBootLRT A data frame including values of the Bartlett-corrected likelihood ratio chi2

statistic, its degrees of freedom, and its p-value;

bootInfo a list with the following elements:

**bootreps** A table of fitted likelihoods for bootstrap replicates;

**meanbootLRT** The mean likelihood ratio chi-square statistic for bootstrap replicates:

When ANOVA tables are computed, the return format is that of the function called (lmerTest::anova for LMMs) or emulated (for LMs or GLMs). For GLMs, by default no test is reported, as has been the default for anova.glm before R 4.4.0.

### References

Bartlett, M. S. (1937) Properties of sufficiency and statistical tests. Proceedings of the Royal Society (London) A 160: 268-282.

Davison A.C., Hinkley D.V. (1997) Bootstrap methods and their applications. Cambridge Univ. Press, Cambridge, UK.

Fai AH, Cornelius PL (1996). Approximate F-tests of multiple degree of freedom hypotheses in generalised least squares analyses of unbalanced split-plot experiments. Journal of Statistical Computation and Simulation, 54(4), 363-378. doi:10.1080/00949659608811740

#### See Also

See also fixedLRT for a different interface to LRTs,

get\_RLRsim\_args for efficient simulation-based implementation of exact likelihood ratio tests for testing the presence of variance components,

as\_LMLT for the interface to lmerTest::anova,

and summary.HLfit(.,details=list(<true|"Wald">)) for reporting the p-value for each t-statistic in the summary table for fixed effects, either by Student's t distribution, or by the approximation of t^2 distribution by the Chi-squared distribution ("Wald's test").

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```
data("wafers")
## Gamma GLMM with log link
\label{eq:m1} \verb| m1 <- HLfit(y ~ X1+X2+X1*X3+X2*X3+I(X2^2)+(1|batch),family=Gamma(log), \\
           resid.model = ~ X3+I(X3^2) ,data=wafers,method="ML")
m2 \leftarrow update(m1, formula. = \sim . -I(X2^2))
anova(m1,m2) # LRT
## 'anova' (Wald chi-squared tests...) for GLMM or model with a 'resid.model'
anova(m1)
## ANOVA table for GLM
# Gamma example, from McCullagh & Nelder (1989, pp. 300-2), as in 'glm' doc:
clotting <- data.frame(</pre>
    u = c(5,10,15,20,30,40,60,80,100),
    lot1 = c(118, 58, 42, 35, 27, 25, 21, 19, 18),
    lot2 = c(69, 35, 26, 21, 18, 16, 13, 12, 12))
spglm \leftarrow fitme(lot1 \sim log(u), data = clotting, family = Gamma, method="REML")
anova(spglm, test = "F")
anova(spglm, test = "Cp")
anova(spglm, test = "Chisq")
anova(spglm, test = "Rao")
## ANOVA table for LMM
if(requireNamespace("lmerTest", quietly=TRUE)) {
  lmmfit < fitme(y \sim X1+X2+X1*X3+X2*X3+I(X2^2)+(1|batch), data=wafers)
  print(anova(lmmfit)) # => Satterthwaite method, here giving p-values
                        # quite close to traditional t-tests given by:
  summary(lmmfit, details=list(p_value=TRUE))
}
## Using resp_testfn argument for bootstrap LRT:
## Not run:
set.seed(1L)
d \leftarrow data.frame(success = rbinom(10, size = 1, prob = 0.9), x = 1:10)
xx \leftarrow cbind(1,d$x)
table(d$success)
m_x <- fitme(success ~ x, data = d, family = binomial())</pre>
m_0 <- fitme(success ~ 1, data = d, family = binomial())</pre>
# Bootstrap LRTs:
anova(m_x, m_0, boot.repl = 100,
      resp_testfn=function(y) {! is_separated(xx,as.numeric(y),verbose=FALSE)})
## End(Not run)
#### Various cases were asymptotic tests may be unreliable:
set.seed(123)
dat <- data.frame(g = rep(1:10, e = 10), x = (x<-rnorm(100)),
                    y = 0.1 * x + rnorm(100)
```

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```
m0 <- fitme(y ~ 1, data=dat)</pre>
## (1) Models differing both by fixed and random effects:
# (note the warning for variance at boundary):
if (spaMM.getOption("example_maxtime")>11) {
  m \leftarrow fitme(y \sim x + (1|g), data=dat)
  LRT(m,m0, boot.repl = 199L)
}
## See help("get_RLRsim_args") for a fast and accurate test procedure
## (2) Models differing also by residual-dispersion models:
if (spaMM.getOption("example_maxtime")>25) {
  m \leftarrow fitme(y \sim x + (1|g), data=dat, resid.model= \sim x)
  LRT(m,m0, boot.repl = 99L)
}
## (3) Models differing (also) by their random-effects in resid.model:
m \leftarrow fitme(y \sim x, data=dat, resid.model= \sim 1+(1|g))
LRT(m,m0) # no test performed
```

make\_scaled\_dist

Scaled distances between unique locations

#### **Description**

This function computes scaled distances from whichever relevant argument it can use (see Details). The result can directly by used as input for computation of the Matérn correlation matrix. It is usually called internally by HLCor, so that users may ignore it, except if they wish to control the distance used through control.dist\$method, or the parametrization of the scaling through control.dist\$rho.mapping.control.dist\$method provide access to the distances implemented in the proxy package, as well as to "EarthChord" and "Earth" methods defined in spaMM (see Details).

## Usage

#### **Arguments**

uniqueGeo

A matrix of geographical coordinates (e.g. 2 columns for latitude and longitude), without replicates of the same location.

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uniqueGeo2 NULL, or a second matrix of geographical coordinates, without replicates of the

same location. If NULL, scaled distances among uniqueGeo locations are computed. Otherwise, scaled distances between locations in the two input matrices

are computed.

distMatrix A distance matrix.

rho A scalar or vector of positive values. Scaled distance is computed as <distances

in each coordinate> \* rho, unless a non-trivial rho.mapping is used.

rho.mapping A set of indices controlling which elements of the rho scale vector scales which

dimension(s) of the space in which (spatial) correlation matrices of random effects are computed. Scaled distance is generally computed as <distances in each coordinate> \* rho[rho.mapping]. As shown in the Example, if one wishes to combine isotropic geographical distance and some environmental distance, the coordinates being latitude, longitude and one environmental variable, the scaled distance may be computed as (say) (lat,long,env) \*rho[c(1,1,2)] so that the same scaling rho[1] applies for both geographical coordinates. In this case, rho should have length 2 and rho.mapping should be c(1,1,2).

dist.method method argument of proxy::dist function (by default, "Euclidean", but other

distances are possible (see Details).

return\_matrix Whether to return a matrix rather than a proxy::dist or proxy::crossdist

object.

#### **Details**

The function uses the distMatrix argument if provided, in which case rho must be a scalar. Vectorial rho (i.e., different scaling of different dimensions) is feasible only by providing uniqueGeo.

The dist.method argument gives access to distances implemented in the proxy package, or to user-defined ones that are made accessible to proxy through its database. Of special interest for spatial analyses are distances computed from longitude and latitude (proxy implements "Geodesic" and "Chord" distances but they do not use such coordinates: instead, they use Euclidean distance for 2D computations, i.e. Euclidean distance between points on a circle rather than on a sphere). spaMM implements two such distances: "Earth" and "EarthChord", using longitude and latitude inputs in that order (see Examples). The "EarthChord" distance is the 3D Euclidean distance "through Earth". The "Earth" distance is also known as the orthodromic or great-circle distance, on the Earth surface. Both distances return values in km and are based on approximating the Earth by a sphere of radius 6371.009 km.

#### Value

A matrix or dist object. If there are two input matrices, rows of the return value correspond to rows of the first matrix.

mapMM

Colorful plots of predictions in two-dimensional space.

### **Description**

These functions provide either a map of predicted response in analyzed locations, or a predicted surface. mapMM is a straightforward representation of the analysis of the data, while filled.mapMM uses interpolation to cope with the fact that all predictor variables may not be known in all locations on a fine spatial grid. map\_ranef maps a single spatial random effect. These three functions takes an HLfit object as input. mapMM calls spaMMplot2D, which is similar but takes a more conventional (x,y,z) input.

Using filled.mapMM may involve questionable choices. Plotting a filled contour generally requires prediction in non-observed locations, where predictor variables used in the original data analysis may be missing. In that case, the original model formula cannot be used and an alternative model (controlled by the map.formula argument) must be used to interpolate (not smooth) the predicted values in observed locations (these predictions still resulting from the original analysis based on predictor variables). filled.mapMM always performs such interpolation (it does not allow one to provide values for the predictor variables). As a result (1) filled.mapMM will be slower than a mere plotting function, since it involves the analysis of spatial data; (2) the results may have little useful meaning if the effect of the original predictor variables is not correctly represented by this interpolation step. For example, prediction by interpolation may be biased in a way analogous to prediction of temperature in non-observed locations while ignoring effect of variation in altitude in such locations. Likewise, the variance argument of filled.mapMM allows one only to plot the prediction variance of its own interpolator, rather than that of the input object.

map\_ranef is free of the limitations of filled.mapMM.

#### Usage

```
spaMMplot2D(x, y, z, xrange=range(x, finite = TRUE),
   yrange=range(y, finite = TRUE), margin=1/20, add.map= FALSE,
   nlevels = 20, color.palette = spaMM.colors, map.asp=NULL,
   col = color.palette(length(levels) - 1), plot.title=NULL, plot.axes=NULL,
   decorations=NULL, key.title=NULL, key.axes=NULL, xaxs = "i",
   yaxs = "i", las = 1, axes = TRUE, frame.plot = axes, ...)

mapMM(fitobject,Ztransf=NULL,coordinates,
   add.points,decorations=NULL,plot.title=NULL,plot.axes=NULL,envir=-3, ...)

filled.mapMM(
```

```
fitobject, Ztransf = NULL, coordinates, xrange = NULL, yrange = NULL,
margin = 1/20, map.formula, phi = 1e-05, gridSteps = 41,
decorations = quote(points(pred[, coordinates], cex = 1, lwd = 2)),
add.map = FALSE, axes = TRUE, plot.title = NULL, plot.axes = NULL,
map.asp = NULL, variance = NULL, var.contour.args = list(),
smoothObject = NULL, return.="smoothObject", ...)

map_ranef(fitobject, re.form, Ztransf=NULL, xrange = NULL, yrange = NULL,
margin = 1/20, gridSteps = 41,
decorations = quote(points(fitobject$data[, coordinates], cex = 1, lwd = 2)),
add.map = FALSE, axes = TRUE, plot.title=NULL, plot.axes=NULL,
map.asp = NULL, ...)
```

### **Arguments**

fitobject The return object of a corrHLfit or fitme call.

x, y, z Three vectors of coordinates, with z being expectedly the response.

re.form A model formula giving the single random effect term to plot, needed only if there are several spatial random effects in the fitted model. In that case, it must

be formatted as . ~ <term>, as for the re.form argument of predict.HLfit.

Ztransf A transformation of the predicted response, given as a function whose only required argument can be a one-column matrix. The name of this argument must

be Z (not x), as is appropriate for use in do.call(Ztransf,list(Z=Zvalues)).

coordinates The geographical coordinates. By default they are deduced from the model for-

mula. For example if this formula is  $resp \sim 1 + Matern(1 \mid x + y)$  the default coordinates are c("x","y"). If this formula is  $resp \sim 1 + Matern(1 \mid x + y + z)$ ,

the user must choose two of the three coordinates.

xrange The x range of the plot (a vector of length 2); by default defined to cover all

analyzed points.

yrange The y range of the plot (a vector of length 2); by default defined to cover all

analyzed points.

margin This controls how far (in relative terms) the plot extends beyond the x and y

ranges of the analyzed points, and is overriden by explicit xrange and yrange

arguments.

map.formula NULL, or a formula whose left-hand side is ignored. Provides the formula used

for interpolation. If NULL, a default formula with the same spatial effect(s) as

in the input fitobject is used.

phi This controls the phi value assumed in the interpolation step. Ideally phi would

be zero, but problems with numerically singular matrices may arise when phi is

too small.

gridSteps The number of levels of the grid of x and y values

variance Either NULL, or the name of a component of variance of prediction by the in-

*terpolator* to be plotted. Must name one of the components that can be returned by predict.HLfit. variance="predVar" is suitable for uncertainty in point

prediction.

var.contour.args

A list of control parameters for rendering of prediction variances. See contour

for possible arguments (except x, y, z and add).

add.map Either a boolean or an explicit expression, enclosed in quote (see Examples).

If TRUE, the map function from the maps package (which much therefore the loaded) is used to add a map from its default world database. xrange and yrange are used to select the area, so it is most convenient if the coordinates are longitude and latitude (in this order and in standard units). An explicit ex-

pression can also be used for further control.

levels a set of levels which are used to partition the range of z. Must be strictly increas-

ing (and finite). Areas with z values between consecutive levels are painted with

the same color.

nlevels if levels is not specified, the range of z, values is divided into \*approximately\*

this many levels (a call to pretty determines the actual number of levels).

color.palette a color palette function to be used to assign colors in the plot.

map.asp the y/x aspect ratio of the 2D plot area (not of the full figure including the scale).

By default, the scales for x and y are identical unless the x and y ranges are too different. Namely, the scales are identical if (plotted y range)/(plotted x range)

is 1/4 < . < 4, and map.asp is 1 otherwise.

col an explicit set of colors to be used in the plot. This argument overrides any

palette function specification. There should be one less color than levels

plot.title statements which add titles to the main plot. See Details for differences between

functions.

plot.axes statements which draw axes (and a box) on the main plot. See Details for differ-

ences between functions.

decorations Either NULL or Additional graphic statements (points, polygon, etc.), en-

closed in quote (the default value illustrates the latter syntax). .

add.points Obsolete, use decorations instead.

envir Controls the environment in which plot.title, plot.axes, and decorations

are evaluated. mapMM calls spaMM2Dplot from where these graphic arguments are evaluated, and the default value -3 means that they are evaluated within the

environment from where mapMM was called.

key.title statements which add titles for the plot key. key.axes statements which draw axes on the plot key.

the x axis style. The default is to use internal labeling.
yaxs the y axis style. The default is to use internal labeling.

las the style of labeling to be used. The default is to use horizontal labeling.

axes, frame.plot

logicals indicating if axes and a box should be drawn, as in plot.default.

smoothObject Either NULL, or an object inheriting from class HLfit (hence, an object on

which  $\operatorname{predict}.\operatorname{HLfit}$  can be called),  $\operatorname{predicting}$  the response surface in any

coordinates. See Details for typical usages.

return. character string: see Value

further arguments passed to or from other methods. For mapMM, all such arguments are passed to spaMMplot2D; for spaMMplot2D, currently only additional graphical parameters passed to title() (see Details). For filled.mapMM and map\_ranef, these parameters are those that can be passed to spaMM.filled.contour.

#### **Details**

The smoothObject argument may be used to redraw a figure faster by recycling the predictor of the response surface returned invisibly by a previous call to filled.mapMM.

For smoothObject=NULL (the default), filled.mapMM interpolates the predicted response, with sometimes unpleasant effects. For example, if one interpolates probabilities, the result may not be within [0,1], and then (say) a logarithmic Ztransf may generate NaN values that would otherwise not occur. The smoothObject argument may be used to overcome the default behaviour, by providing an alternative predictor.

If you have values for all predictor variables in all locations of a fine spatial grid, filled.mapMM may not be a good choice, since it will ignore that information (see map.formula argument). Rather, one should use predict(<fitobject>,newdata= <all predictor variables >) to generate all predictions, and then either spaMM. filled.contour or some other raster functions.

The different functions are (currently) inconsistent among themselves in the way they handle the plot.title and plot.axes argument:

**spaMM.filled.contour** behaves like graphics::filled.contour, which (1) handles arguments which are calls such as title(.) or {axis(1);axis(2)}; (2) ignores . . . arguments if plot.title is missing; and (3) draws axes by default when plot.axes is missing, given axes = TRUE.

By contrast, **filled.mapMM** handles arguments which are language expressions such as produced by quote(.) or substitute(.) (see Examples).

mapMM can handles language expressions, but also accepts at least some calls.

### Value

filled.mapMM by default returns invisibly the fit object predicting the interpolated response surface; however, for any non-default return. argument (return.="raster" would be recommended to ensure future back-compatibility), it will return a raster of values as a list with elements x, y and z. map\_ranef returns invisibly a 3-column matrix containing the spatial coordinates, and the predicted effect z on the linear predictor scale (which is also the scale of the plot, unless a Ztransf is used). mapMM returns invisibly a list with elements x, y and z. Plots are produced as side-effects.

#### See Also

seaMask for masking areas in a filled map; https://gitlab.mbb.univ-montp2.fr/francois/spamm-ref/-/blob/master/vignettePlus/example\_raster.html for more elaborate plot procedures.

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```
map_ranef(bfit) # providing argument re.form= . ~ Matern(1|longitude+latitude)
if (spaMM.getOption("example_maxtime")>1) {
 ## filled.mapMM takes a bit longer
 # showing 'add.map', 'nlevels', and contour lines for 'variance'
 filled.mapMM(bfit, nlevels=30, add.map=TRUE, plot.axes=quote({axis(1);axis(2)}),
             variance="respVar",
             plot.title=title(main="Inferred migration propensity of blackcaps",
                                xlab="longitude",ylab="latitude"))
  ## Similar plots by ggplot2:
 ## Not run:
  library(rnaturalearth) # provides sea mask through 'ne_download' function
  library(ggplot2)
  library(sp)
   # sea mask
  sea <- ne_download(scale = 10, type = 'ocean', category = "physical", returnclass = "sf")</pre>
  # Generation of data.frame for ggplot:
  rastr <- filled.mapMM(bfit, return.="raster")</pre>
  spdf <- data.frame(Long=rep(rastr$x, nc), Lat=rastr$y[gl(nr,nc)], z = as.vector(rastr$z))</pre>
   ggplot(spdf) +
     geom_contour_filled(aes(Long,Lat,z=z), bins = 20) +
     guides(fill = "none") +
     geom_sf(data = sea, fill = "black") +
     coord_sf(ylim = range(rastr$y), xlim = range(rastr$x), expand = FALSE)
## End(Not run)
}
if (spaMM.getOption("example_maxtime")>3) {
data("Loaloa")
lfit <- fitme(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI</pre>
                  + {\tt Matern(1|longitude+latitude),\ method="PQL",\ data=Loaloa,}\\
                  family=binomial(), fixed=list(nu=0.5,rho=2.255197,lambda=1.075))
 ## longer computation requiring interpolation of 197 points
 ## Also illustrating effect of 'return.' argument
 res <- filled.mapMM(lfit,add.map=TRUE,plot.axes=quote({axis(1);axis(2)}),</pre>
    decorations=quote(points(pred[,coordinates],pch=15,cex=0.3)),
    return.="raster", # so that 'res' is a list representing a raster.
   plot.title=title(main="Inferred prevalence, North Cameroon",
                     xlab="longitude",ylab="latitude"))
}
```

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### **Description**

The Matérn correlation function describes realizations of Gaussian spatial processes with different smoothnesses (i.e. either smooth or rugged surfaces, controlled by the  $\nu$  parameter). It also includes a  $\rho$  scaling parameter and an optional 'nugget' parameter. A random effect specified in a model formula as Matern(1|<...>) has pairwise correlations given by the Matérn function at the scaled Euclidean distance between coordinates specified in <...>, using "+" as separator (e.g., Matern(1|longitude+latitude)). The Matern family can be used in Euclidean spaces of any dimension; and also for correlations on a sphere (with maximum smoothness nu=0.5).

A syntax of the form Matern(1|longitude+latitude %in% grp) can be used to specify a Matern random effect with independent realizations (but identical correlation parameters) for each level of the grouping variable grp. Alternatively, the Matern(<T/F factor>|longitude+latitude) may be used to specify Matern effects specific to individuals identified by the <T/F factor> (see Example with females and males). In that case distinct correlation parameters are fitted for each such Matern term.

When group-specific autocorrelated random effects are fitted, it may be wise to allow for different means for each group in the Intercept (a message will point this out if the fit results for Matern or Cauchy terms suggest so).

By default, fitme and corrHLfit performs optimization over the  $\rho$  and  $\nu$  parameters. It is possible to estimate different scaling parameters for the different Euclidean dimensions: see examples in make\_scaled\_dist.

The MaternCorr function may be used to vizualise these correlations, using distances as input.

#### Usage

```
## Default S3 method:
MaternCorr(d, rho = 1, smoothness, nu = smoothness, Nugget = NULL)
# Matern(1|...)
```

formatting is required.

### **Arguments**

d	A distance or a distance matrix.
rho	A scaling factor for distance. The 'range' considered in some formulations is the reciprocal of this scaling factor
smoothness	The smoothness parameter, >0. $\nu=0.5$ corresponds to the exponential correlation function, and the limit function when $\mu$ goes to $\infty$ is the squared exponential function (as in a Gaussian).
nu	Same as smoothness
Nugget	(Following the jargon of Kriging) a parameter describing a discontinuous decrease in correlation at zero distance. Correlation will always be 1 at $d=0$ , and from which it immediately drops to (1-Nugget)
	Names of coordinates, using "+" as separator (e.g., Matern(1 longitude+latitude). The coordinates are numeric values found in the data data frame provided to the

fitting function. No additional declaration of groups, factors, or other specific

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#### **Details**

The correlation at distance d > 0 is

$$(1-{\rm Nugget})\frac{(\rho d)^{\nu}K_{\nu}(\rho d)}{2^{(\nu-1)}\Gamma(\nu)}$$

where  $K_{\nu}$  is the besselK function of order  $\nu$ .

By default the Nugget is set to 0. See one of the examples on data set Loaloa for a fit including the estimation of the Nugget.

#### Value

Scalar/vector/matrix depending on input.

#### References

Stein, M.L. (1999) Statistical Interpolation of Spatial Data: Some Theory for Kriging. Springer, New York.

#### See Also

See corMatern for an implementation of this correlation function as a corSpatial object for use with lme or glmmPQL.

```
## See examples in help("HLCor"), help("Loaloa"), help("make_scaled_dist"), etc.
## Matern correlations in 4-dimensional space:
set.seed(123)
randpts <- matrix(rnorm(20),nrow=5)</pre>
distMatrix <- as.matrix(proxy::dist(randpts))</pre>
MaternCorr(distMatrix,nu=2)
## Group-specific random effects:
if (spaMM.getOption("example_maxtime")>1.6) {
  data(Leuca)
 subLeuca < - Leuca[c(1:10,79:88),] # subset of 10 females and 10 males, for faster examples.
  # Independent Matern random effect with different covariance parameters for each sex:
  fitme(fec_div \sim sex + Matern(female|x + y) + Matern(male|x + y), data = subLeuca)
  # Independent Matern random effect with the same covariance parameters for each sex:
  fitme(fec_div ~ sex + Matern(1|x+y %in% sex),data=subLeuca)
  # Matern models with random-effects distinct but correlated across sexes
  # can also be fitted: see Matern examples in help("composite-ranef").
}
```

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model.	MaternIMRFa	corrFamily constructor for Interpolated Markov Random Field (IMRF) covariance structure approximating a 2D Matern correlation model.
--------	-------------	--

## **Description**

Reimplements the IMRF correlation model approximating a Matern correlation function, through a corrFamily constructor. This allows the efficient joint estimation of the alpha parameter of the approximating Markov random field (in principle related to the smoothness parameter of the Matern correlation function) together with its kappa parameter. By contrast, random effects terms specified as IMRF(1|., model = <INLA::inla.spde2.matern result>) assume a fixed alpha.

Using this feature requires that the not-on-CRAN package INLA (https://www.r-inla.org) is installed so that INLA::inla.spde2.matern can be called for each alpha value.

### Usage

```
# corrFamily constructor:
MaternIMRFa(mesh, tpar = c(alpha = 1.25, kappa = 0.1), fixed = NULL, norm=FALSE)
```

## **Arguments**

mesh An inla.mesh object as produced by INLA::inla.mesh.2d.

and consistently with the general format of corrFamily constructors:

tpar Named numeric vector: template values of the parameters of the model. Better not modified unless you know what you are doing.

fixed NULL or numeric vector, to fix the parameters of this model.

norm Boolean: whether to apply a normalization so that the random effect is homoscedastic (see IMRF) for details.

## Value

A list suitable as input in the covStruct argument, with the following elements:

f	function returning a precision matrix for the random effect in mesh vertices;
tpar	template parameter vector (see general requirements of a corrFamily descriptor);
Af	function returning a matrix that implements the prediction of random effect values in data locations by interpolation of values in mesh locations (similarly to INLA::inla.spde.make.A);
type	specifies that the matrix returned by Cf is a precision matrix rather than a correlation matrix;

and possibly other elements which should not be considered as stable features of the return value.

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#### References

Lindgren F., Rue H., Lindström J. (2011) An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach Journal of the Royal Statistical Society: Series B (Statistical Methodology), 73: 423-498. doi:10.1111/j.1467-9868.2011.00777.x

```
## Not run:
if(requireNamespace("INLA", quietly = TRUE)) {
data("Loaloa")
mesh <- INLA::inla.mesh.2d(loc = Loaloa[, c("longitude", "latitude")],</pre>
                     \max.edge = c(3, 20)
### Fit with fixed alpha
(fit_MaternIMRF <- fitme(</pre>
 cbind(npos,ntot-npos) ~ elev1 + elev2 + elev3 + elev4 + maxNDVI1 +
        seNDVI + MaternIMRFa(1|longitude+latitude, mesh, fixed=c(alpha=1.05)),
 family=binomial(),
 data=Loaloa, verbose=c(TRACE=interactive())) )
# For data sets with a small number of locations (as here), fitting
# the Matern model as follows is faster than fitting its MaternIMRFa approximation.
# Here this appears more than twofold faster
fit_Matern <- fitme(</pre>
 cbind(npos,ntot-npos) ~ elev1 + elev2 + elev3 + elev4 + maxNDVI1 +
        seNDVI + Matern(1|longitude+latitude),
 fixed=list(nu=0.05),
                                                 # in principle similar to alpha=0.05
 data=Loaloa,family=binomial())
### Same with variable alpha
(fit_MaternIMRF <- fitme(</pre>
 cbind(npos,ntot-npos) ~ elev1 + elev2 + elev3 + elev4 + maxNDVI1 +
        seNDVI + MaternIMRFa(1|longitude+latitude, mesh),
 family=binomial(),
 data=Loaloa, verbose=c(TRACE=interactive())) )
# Comparable Matern fit:
fit_Matern <- fitme(</pre>
 cbind(npos,ntot-npos) ~ elev1 + elev2 + elev3 + elev4 + maxNDVI1 +
        seNDVI + Matern(1|longitude+latitude),
 init=list(nu=0.25), lower=list(nu=0), upper=list(nu=1),
 data=Loaloa,family=binomial())
```

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```
# Note that the fitted nu and alpha parameters do not quite match each other,
# and that the IMRF likelihood does not really approximate the Matern likelihood.
# Mesh design would also be seen to matter.
} else print("INLA must be installed to run this example.")
## End(Not run)
```

mat\_sqrt

Computation of "square root" of symmetric positive definite matrix

### Description

mat\_sqrt is not usually directly called by users, but arguments may be passed to it through higher-level calls (see Examples). For given matrix  $\mathbf{C}$ , it computes a factor  $\mathbf{L}$  such that  $\mathbf{C} = \mathbf{L} * t(\mathbf{L})$ , handling issues with nearly-singular matrices. The default behavior is to try Cholesky factorization, and use eigen if it fails. Matrix roots are not unique (for example, they are lower triangular for t(chol(.)), and symmetric for svd(.). As matrix roots are used to simulate samples under the fitted model (in particular in the parametric bootstrap implemented in fixedLRT), this implies that for given seed of random numbers, these samples will differ with these different methods (although their distribution should be identical).

### Usage

```
mat_sqrt(m = NULL, symSVD = NULL, try.chol = TRUE, condnum=1e12)
```

previous versions).

# Arguments

m	The matrix whose 'root' is to be computed. This argument is ignored if symSVD is provided.
symSVD	A list representing the symmetric singular value decomposition of the matrix which 'root' is to be computed. Must have elements \$u, a matrix of eigenvectors, and \$d, a vector of eigenvalues.
try.chol	If try.chol=TRUE, the Cholesky factorization will be tried.
condnum	(large) numeric value. In the case cho1() was tried and failed, the matrix is regularized so that its (matrix 2-norm) condition number is reduced to condnum (in version 3.10.0 this correction has been implemented more exactly than in

## Value

For non-NULL m, its matrix root, with rows and columns labelled according to the columns of the original matrix. If eigen was used, the symmetric singular value decomposition (a list with members u (matrix of eigenvectors) and d (vector of eigenvalues)) is given as attribute.

method

## **Examples**

method

Fitting methods (objective functions maximized)

### Description

The method argument of the fitting functions, with possible values "ML", "REML", "PQL", "PQL/L", and so on, controls whether restricted likelihood techniques are used to estimate residual variance and random-effect parameters, and the way likelihood functions are approximated.

By default, Laplace approximations are used, as selected by "ML" and "REML" methods. The Laplace approximation to (log-)marginal likelihood can be expressed in terms of the joint log-likelihood of the data and the random effects (or the *h*-likelihood in works of Lee and Nelder). The Laplace approximation is the joint likelihood minus half the log-determinant of the matrix of second derivatives (Hessian matrix) of the negative joint likelihood with respect to the random effects (observed information matrix). The Laplace approximation to restricted likelihood (for REML estimation) is similarly defined from the Hessian matrix with respect to random effects **and** fixed effects (for the adventurous, **spaMM** allows some non-standard specification of the fixed effects included in the definition of he Hessian).

Various additional approximations have been considered. Penalized quasi-likelihood (PQL), as originally defined for GLMMs by Breslow and Clayton (1993), uses a Laplace approximation of restricted likelihood to estimate dispersion parameters, and estimates fixed effects by maximizing the joint likelihood (h-likelihood). Although PQL has been criticized as an approximation of likelihood (and actual implementations may diverge from the original version), it has some interesting inferential properties. **spaMM** allows one to use an ML variant of PQL, named PQL/L.

Further approximations defined by Lee, Nelder and collaborators (e.g., Noh and Lee, 2007, for some overview) may mostly be seen as laying between PQL and the full Laplace method in terms of approximation of the likelihood, and as extending them to models with non-gaussian random effects ("HGLMs"). In practice the ML, REML, PQL and PQL/L methods should cover most (all?) needs for GLMMs, and EQL extends the PQL concept to HGLMs. method="EQL+" stands for the EQL method of Lee and Nelder (2001). The '+' signals that it includes the d v/d tau correction described p. 997 of that paper, while method="EQL-" ignores it. "PQL" is equivalent to EQL- for GLMMs. "PQL/L" is PQL without the leverage corrections that characterize REML estimation of random-effect parameters.

spaMM uses the observed information matrix by default since version 4.0.0. By contrast, in Laplace approximations of likelihood described in the work of Lee & Nelder, i.e. for mixed-effect models with GLM response families, the information matrix is written in terms of the GLM weights (e.g., Lee & Nelder 2001, p.1004), and is thus effectively the expected information matrix, which differs from the observed information matrix in the case of GLM families with non-canonical link (McCullagh & Nelder 1989, p.42). Therefore, the likelihood approximation based on the expected information matrix differs from the one based on the observed information matrix in the same conditions.

For non-GLM response families (currently, the negbin1, beta\_resp and betabin), only observed information is available (expected information would at best be quite difficult to evaluate, with no benefits). For GLM response families, use of expected information matrix can be required at a global level by setting spaMM.options(obsInfo=FALSE) or in a specific fit by adding "exp" as a second specifier in the method (e.g., method=c("ML", "exp")). This can be distinctly useful (in terms of speed) for fitting models with Gamma(log) response family. Conversely, the "obs" specifier will enforce use of observed information matrix when the alternative is set at a global level.

#### **Details**

The method (or HLmethod) argument of fitting functions also accepts values of the form "HL(<...>)", "ML(<...>)" and "RE(<...>)", e.g. method="RE(1,1)", which allow one to experiment with further combinations of approximations. HL and RE are equivalent (both imply an REML correction). The first '1' means that a Laplace approximation to the likelihood is used to estimate fixed effects (a '0' would instead mean that the h likelihood is used as the objective function). The second '1' means that a Laplace approximation to the likelihood or restricted likelihood is used to estimate dispersion parameters, this approximation including the dv/d tau term specifically discussed by Lee & Nelder 2001, p. 997 (a '0' would instead mean that these terms are ignored). It is possible to enforce the EQL approximation for estimation of dispersion parameter (i.e., Lee and Nelder's (2001) method) by adding a third index with value 0. "EQL+" is thus "HL(0,1,0)", while "EQL-" is "HL(0,0,0)". "PQL" is EQL- for GLMMs. "REML" is "HL(1,1)". "ML" is "ML(1,1)".

Some of these distinctions make sense for **GLMs**, and may help in understanding idiosyncrasies of stats::glm for Gamma GLMs. In particular (as stated in the stats::logLik documentation) the logLik of a Gamma GLM fit by glm differs from the exact likelihood. An "ML(0,0,0)" approximation of true ML provides the same log likelihood as stats::logLik. Further, the dispersion estimate returned by summary.glm differs from the one implied by logLik, because summary.glm uses Pearson residuals instead of deviance residuals. This may be confusing, and no method in **spaMM** tries to reproduce simultaneously these distinct features (however, spaMM\_glm may do so). The dispersion estimate returned by an "HL(.,.,0)" fit matches what can be computed from residual deviance and residual degrees of freedom of a glm fit, but this is not the estimate displayed by summary.glm. The fixed effect estimates are not affected by these tinkerings.

## References

Breslow, NE, Clayton, DG. (1993). Approximate Inference in Generalized Linear Mixed Models. Journal of the American Statistical Association 88, 9-25.

Lee, Y., Nelder, J. A. (2001) Hierarchical generalised linear models: A synthesis of generalised linear models, random-effect models and structured dispersions. Biometrika 88, 987-1006.

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McCullagh, P. and Nelder, J.A. (1989) Generalized Linear Models, 2nd edition. London: Chapman & Hall.

Noh, M., and Lee, Y. (2007). REML estimation for binary data in GLMMs, J. Multivariate Anal. 98, 896-915.

**MSFDR** 

Multiple-Stage False Discovery Rate procedure

## **Description**

This implements the procedure described by Benjamini and Gavrilov (2009) for model-selection of fixed-effect terms based on False Discovery Rate (FDR) concepts. It uses forward selection based on penalized likelihoods. The penalization for the number of parameters is distinct from that in Akaike's Information Criterion, and variable across iterations of the algorithm (but functions from the stats package for AIC-based model-selection are still called, so that some screen messages refer to AIC).

## Usage

```
MSFDR(nullfit, fullfit, q = 0.05, verbose = TRUE)
```

## **Arguments**

nullfit	An ML fit to the minimal model to start the forward selection from; an object of class HLfit.
fullfit	An ML fit to the maximal model; an object of class HLfit.
q	Nominal error rate of the underlying FDR procedure (expected proportion of incorrectly rejected null out of the rejected). Benjamini and Gavrilov (2009) recommend q=0.05 on the basis of minimizing mean-squared prediction error in various simulation conditions considering only linear models.
verbose	Whether to print information about the progress of the procedure.

## Value

The fit of the final selected model; an object of class HLfit.

### References

A simple forward selection procedure based on false discovery rate control. Ann. Appl. Stat, 3, 179-198 (2009).

```
if (spaMM.getOption("example_maxtime")>1.4) {
  data("wafers")
nullfit <- fitme(y~1+(1|batch), data=wafers,family=Gamma(log))
fullfit <- fitme(y ~X1+X2+X1*X3+X2*X3+I(X2^2)+(1|batch), data=wafers, family=Gamma(log))
MSFDR(nullfit=nullfit,fullfit=fullfit)
}</pre>
```

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multIMRF	Interpolated Markov Random Field models

### Description

**spaMM** can fit random-effect terms of the forms considered by Lindgren et al. (2011) or Nychka et al. (2015, 2018). The random effects considered here all involve a multivariate Gaussian random effect over a lattice, from which the random-effect value in any spatial position is determined by interpolation of values on the lattice. **IMRF** stands for Interpolated Markov Random Field because the specific process considered on the lattice is currently known as a Gaussian Markov Random Field (see the Details for further information). Lindgren et al. considered irregular lattices designed to approximate of the Matern correlation model with fixed smoothness <= 2, while Nychka et al. considered regular grids.

The correlation model of Lindgren et al. (2011) can be fitted by **spaMM** by declaring an IMRF random effect term in the model formula, with a model argument in the right-hand side whose value is the result of INLA::inla.spde2.matern (or INLA::inla.spde2.pcmatern) for given smoothness. The **spaMM** functions for such a fit do not call **INLA** functions. Alternatively, the same model with variable smoothness can be fitted by declaring a corrFamily term whose structure is described through the MaternIMRFa function, whose respective documentations should be considered for more details. In the latter case INLA::inla.spde2.matern is called internally by spaMM. The correlation models thus defined are fitted by the same methods as other models in **spaMM**.

Regular lattices can also be declared as an IMRF term (with arguments distinct from model). The multIMRF syntax implements the multiresolution model of Nychka et al. Any multIMRF term in a formula is immediately converted to IMRF terms for regular grids wih different step sizes. This has distinct implications for controlling the parameters of these or other random effects in the model by init or fixed values: see Details if you need such control.

### Usage

# Arguments

mode1	An inla.spde2 object as produced by INLA::inla.spde2.matern or INLA::inla.spde2.pcmatern (see Examples below, and https://www.r-inla.org for further information).
levels	integer; Number of levels in the hierarchy, i.e. number of component IMRFs.
margin, m	integer; width of the margin, as a number of additional grid points on each side (applies to all levels of the hierarchy).
coarse	integer; number of grid points (excluding the margins) per dimension for the coarsest IMRF. The number of grids steps nearly doubles with each level of the hierarchy (see Details).

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nd integer; number of grid steps (excluding the margins) per dimension for the

given IMRF.

norm, no Boolean; whether to apply normalization (see Details), or not. centered, ce Boolean; whether to center the grid in all dimensions, or not.

. . . Not documented, for programming purposes

#### **Details**

### Formulation of the covariance models:

Gaussian Markov Random Field (MRF) and conditional autoregressive models are essentially the same thing, apart from details of specification. adjacency and AR1 random effects can be seen as specific MRFs. The common idea is the Markov-like property that the distribution of each element  $b_i$  of the random-effect  $\mathbf{b}$ , given values of a few specific elements (the "neighbours" of i), is independent of other elements (i.e., of non-neighbours). The non-zero non-diagonal elements of a precision matrix characterize the neighbours.

Given the inferred vector **b** of values of the MRF on the lattice, the interpolation of the MRF in any focal point is of the form **Ab** where each row of **A** weights the values of **b** according to the position of the focal point relative to the vertices of the lattice. Following the original publications,

- \* for grids given by model=<inla.spde2 object>, the non-zero weights are the barycentric coordinates of the focal point in the enclosing triangle from the mesh triangulation (points from outside the mesh would have zero weights, so the predicted effect **Ab=0**);
- \* for regular grids (NULL model), the weights are computed as <Wendland function>(<scaled Euclidean distances between focal point and vertices>).

The IMRF model defines both a lattice in space, the precision matrix for a Gaussian MRF over this lattice, and the **A** matrix of weights. The full specification of the MRF on **irregular lattices** is complex. The  $\kappa$  (kappa) parameter considered by spaMM is the  $\kappa$  scale parameter considered by Lindgren et al and comparable to the  $\rho$  scale factor of the Matérn model. The  $\alpha$  argument of the INLA::inla.spde2.matern controls the smoothness of the approximated Matern model, as  $\alpha = \nu + d/2$ ) where d is the dimension of the space. Correlation models created by INLA::inla.spde2.pcmatern are handled so as to give the same correlation values as when INLA::inla.spde2.matern is used with the same mesh and alpha argument (thus, the extra functionalities of "pc"matern are ignored).

Not all options of the INLA functions may be compatible or meaningful when used with spaMM (only the effects of alpha and cutoff have been checked).

## Normalization:

For the MRFs on default **regular grids** (missing model argument), the precision matrix is defined (up to a variance parameter) as  $\mathbf{M'M}$  where the diagonal elements  $m_{ii}$  of  $\mathbf{M}$  are  $4+\kappa^2$  and the  $m_{ij}$  for the four nearest neighbours are -1 (note that  $\mathbf{M'M}$  involves more than these four neighbours). The precision matrix defined in this way is the inverse of an heteroscedastic covariance matrix  $\mathbf{C}$ , but (following Nychka et al.) by default a normalization is applied so that the random effect in each data position is homoscedastic (the precision matrix for the latent effect in grid positions is not modified, but it is the  $\mathbf{A}$  matrix of weights which is is modified). As for other random effects, the variance is further controlled by a multiplicative factor  $\lambda$ .

Without normalization, the covariance matrix of the random effect in data locations is  $\lambda$ **ALL'A'** (**A** being the above-described weight matrix, and **L** is a "square root" of **C**), and **AL** is the original "design matrix" of the random effect.  $\lambda$  may then be quite different from the marginal variance of

the random effect, and is difficult to describe in a simple way. For normalization, **A** is modified as **WA** where **W** is a diagonal matrix such that **WAL** is a correlation matrix (**WALL'A'W'** has unit diagonal); then,  $\lambda$  is the marginal variance of the random effect.

For irregular grids specified using the model argument, the precision matrix described by this object is also the inverse of an heteroscedastic covariance matrix, but here (again following original publications such as Lindgren at al. 2011) the normalization is not applied by default (and was not even an option before version 4.3.23). But for ease of presentation and interpretation, if for no other reason, the normalized model may be preferable.

### **Details for rectangular grids:**

By default (meaning in particular that model is not used to specify a lattice defined by the INLA procedures), the IMRF lattice is rectangular (currently the only option) and is made of a core lattice, to which margins of margin steps are added on each side. The core lattice is defined as follows: in each of the two spatial dimensions, the range of axial coordinates is determined. The largest range is divided in nd-1 steps, determining nd values and step length L. The other range is divided in steps of the same length L. If it extends over (say) 2.5L, a grid of 2 steps and 3 values is defined, and by default centered on the range (the extreme points therefore typically extend slightly beyond the grid, within the first of the additional steps defined by the margin; if not centered, the grid start from the lower coordinate of the range).

multIMRF implements multilevel IMRFs. It defines a sequence of IMRFs, with progressively finer lattices, a common  $\kappa$  value hy\_kap for these IMRFs, and a single variance parameter hy\_lam that determines  $\lambda$  values decreasing by a factor of 4 for successive IMRF terms. By default, each component IMRF is normalized independently as described above (as in Nychka et al. 2019), and hy\_lam is the sum of the variances of these terms (e.g., if there are three levels and hy\_lam=1, the successive variances are (1,1/4,1/16)/(21/16)). The nd of the first IMRF is set to the coarse value, and its lattice is defined accordingly. If coarse=4 and margin=5, a grid of 14 coordinates is therefore defined over the largest range. In the second IMRF, the grid spacing is halved, so that new steps are defined halfway between the previous ones (yielding a grid of 27 step in the widest range). The third IMRF proceeds from the second in the same way, and so on.

To control initial or fixed values of multIMRF  $\kappa$  and variance parameters, which are hyper-parameter controlling several IMRF terms, the hyper syntax shown in the Examples should be used. hyper is a nested list whose possible elements are named "1", "2", ... referring to successive multIMRF terms in the input formula, not to successive random effect in the expanded formula with distinct IMRF terms (see Examples). But the different IMRF terms should be counted as distinct random effects when controlling other parameters (e.g., for fixing the variances of other random effects).

#### References

- D. Nychka, S. Bandyopadhyay, D. Hammerling, F. Lindgren, S. Sain (2015) A multiresolution gaussian process model for the analysis of large spatial datasets. Journal of Computational and Graphical Statistics 24 (2), 579-599. doi:10.1080/10618600.2014.914946
- D. Nychka, D. Hammerling, Mitchel. Krock, A. Wiens (2018) Modeling and emulation of nonstationary Gaussian fields. Spat. Stat. 28: 21-38. doi:10.1016/j.spasta.2018.08.006

Lindgren F., Rue H., Lindström J. (2011) An explicit link between Gaussian fields and Gaussian Markov random fields: the stochastic partial differential equation approach Journal of the Royal Statistical Society: Series B (Statistical Methodology), 73: 423-498. doi:10.1111/j.1467-9868.2011.00777.x

```
if (spaMM.getOption("example_maxtime")>6) {
data("blackcap") ## toy examples; but IMRF may be useful only for much larger datasets
## and when using the 'cutoff' parameter of INLA::inla.mesh.2d()
################################# Irregular lattice specified by 'model':
data("small_spde") ## load object of class 'inla.spde2', created and saved by :
 # spd <- sp::SpatialPointsDataFrame(coords = blackcap[, c("longitude", "latitude")],</pre>
                                data = blackcap)
 # small_mesh <- INLA::inla.mesh.2d(loc = INLA::inla.mesh.map(sp::coordinates(spd)),</pre>
                              max.n=100, # only for demonstration purposes
                               max.edge = c(3, 20))
 # small_spde <- INLA::inla.spde2.matern(small_mesh)</pre>
 # save(small_spde, file="small_spde.RData", version=2)
fit_SPDE <- fitme(migStatus ~ means + IMRF(1|longitude+latitude, model=small_spde),</pre>
                  data=blackcap)
#################### Regular lattices:
#Using 'hyper' to control fixed hyper-parameters
(mrf \leftarrow fitme(migStatus \sim 1 + (1|pos) +
                          multIMRF(1|longitude+latitude,margin=5,levels=2),
              data=blackcap, fixed=list(phi=1,lambda=c("1"=0.5),
              hyper=list("1"=list(hy_kap=0.1,hy_lam=1)))) )
# Using 'hyper' to control initial hyper-parameters
(mrf <- fitme(migStatus ~ 1 + multIMRF(1|longitude+latitude,margin=5,levels=2),</pre>
                data=blackcap, method="ML", fixed =list(phi=1),
                init=list(hyper=list("1"=list(hy_kap=0.1,hy_lam=1)))) )
# *Independent* IMRF terms with default rectangular lattice (often giving dubious results)
(mrf <- fitme(migStatus ~ 1 + IMRF(1|longitude+latitude,margin=5, nd=4L)</pre>
                               + IMRF(1|longitude+latitude,margin=5, nd=7L),
          data=blackcap,
          fixed=list(phi=1, lambda=c(1/4, 1/16),
                       corrPars=list("1"=list(kappa=0.1),"2"=list(kappa=0.1))))
}
```

### **Description**

These functions facilitate the conversion and analysis of multinomial data as as series of nested binomial data. The main interface is the multi "family", to be used in the family argument of the fitting functions. Fits using it call binomialize, which can be called directly to check how the data are converted to nested binomial data, and to use these data directly. The fitted.HLfitlist method of the fitted generic function returns a matrix of fitted multinomial probabilities. The logLik.HLfitlist method of the logLik generic function returns a log-likelihood for the joint fits.

# Usage

### **Arguments**

data	The data frame to be analyzed.
object	A list of binomial fits returned by a multinomial analysis
responses	column names of the data, such that <data>[,<responses>] contain the multinomial response data, as levels of factor variables.</responses></data>
sortedTypes	Names of multinomial types, i.e. levels of the multinomial response factors. Their order determines which types are taken first to define the nested binomial samples. By default, the most common types are considered first.
binResponse	The names to be given to the number of "success" and "failures" in the binomial response.
depth	The maximum number of nested binomial responses to be generated from the multinomial data.
binfamily	The family applied to each binomial response.
input	If input="types", then the responses columns must contain factor levels of the binomial response. If input="counts", then the responses columns must contain counts of different factor levels, and the column names are the types.
which	Which element of the APHLs list to return. The default depends on the fitting method. In particular, if it was REML or one of its variants, the function returns the log restricted likelihood (exact or approximated).
version	Integer, for fitted.HLfitlist (i.e. for multinomial fits using multi); 1 will provide the result of past versions up to 3.5.0 (See Value).
	Other arguments passed from or to other functions.

#### **Details**

A multinomial response, say counts 17, 13, 25, 8, 3, 1 for types type1 to type6, can be represented as a series of nested binomials e.g. type1 against others (17 vs 50) then among these 50 others, type2 versus others (13 vs 37), etc. The binomialize function generates such a representation. By default the representation considers types in decreasing order of the number of positives, i.e. first type3 against others (25 vs 42), then type1 against others within these 42, etc. It stops if it has reached depth nested binomial responses. This can be modified by the sortedTypes argument, e.g. sortedTypes=c("type6", "type4", "type2"). binomialize returns a list of data frames which can be directly provided as a data argument for the fitting functions, with binomial response.

Alternatively, one can provide the multinomial response data frame, which will be internally converted to nested binomial data if the family argument is a call to multinomial (see Examples).

For mixed models, the multinomial data can be fitted to a model with the same correlation parameters, and either the same or different variances of random effects, for all binomial responses. Which analysis is performed depends on whether the variances are fitted by "outer optimization" or by HLfit's "inner iterative" algorithm, as controlled by the init or init.corrHLfit arguments (see Examples). These initial values therefore affect the definition of the model being fitted. corrHLfit will fit different variances by default. Adding an init.corrHLfit will force estimation of a single variance across models. fitme's default optimization strategy is more complex, and has changed and still change over versions. This creates a **back-compatibility issue** where the model to be fitted may change over versions of spaMM. To avoid that, it is strongly advised to use an explicit initial value when fitting a multi model by fitme.

#### Value

binomialize returns a list of data frames appropriate for analysis as binomial response. Each data frame contains the original one plus two columns named according to binResponse.

The main fitting functions, when called on a model with family=multi(.), return an object of class HLfitlist, which is a list with attributes. The list elements are fits of the nested binomial models (objects of class HLfit). The attributes provide additional information about the overall multinomial model, such as global log-likelihood values and other information properly extracted by the how() function.

multi is a function that returns a list, but users may never need to manipulate this output.

fitted.HLfitlist returns a matrix. The current default version=2L provides meaningful fitted values (predicted multinomial frequencies for each response type) even for data rows where the nested binomial fit for a type had no response information remaining. By contrast, the first version provided a matrix with 0s for these row\*fit combinations, except for the last column; in many cases this may be confusing.

```
head(fitted(colfit))
# To only generate the binomial datasets:
binomialize(iriscol, responses="col")
## An example considering pseudo-data at one diploid locus for 50 individuals
set.seed(123)
genecopy1 <- sample(4,size=50,prob=c(1/2,1/4,1/8,1/8),replace=TRUE)</pre>
genecopy2 <- sample(4,size=50,prob=c(1/2,1/4,1/8,1/8),replace=TRUE)</pre>
alleles <- c("122","124","126","128")
genotypes <- data.frame(type1=alleles[genecopy1],type2=alleles[genecopy2])</pre>
## Columns "type1","type2" each contains an allele type => input is "types" (the default)
datalist <- binomialize(genotypes,responses=c("type1","type2"))</pre>
## two equivalent fits:
f1 <- HLfit(cbind(npos,nneg)~1,data=datalist, family=binomial())</pre>
f2 <- HLfit(cbind(npos,nneg)~1,data=genotypes, family=multi(responses=c("type1","type2")))</pre>
fitted(f2)
if (spaMM.getOption("example_maxtime")>1.7) {
##### Control of lambda estimation over different binomial submodels
genoInSpace <- data.frame(type1=alleles[genecopy1],type2=alleles[genecopy2],</pre>
                           x=runif(50),y=runif(50))
method <- "PQL" # for faster exampple
## Fitting distinct variances for all binomial responses:
multifit <- corrHLfit(cbind(npos,nneg)~1+Matern(1|x+y),data=genoInSpace,</pre>
                      family=multi(responses=c("type1", "type2")),
                      ranFix=list(rho=1,nu=0.5), method=method)
length(unique(unlist(lapply(multifit, get_ranPars, which="lambda")))) # 3
multifit <- fitme(cbind(npos,nneg)~1+Matern(1|x+y),data=genoInSpace,</pre>
                  family=multi(responses=c("type1","type2")),
                  init=list(lambda=NaN), # forcing 'inner' estimation for fitme
                  fixed=list(rho=1,nu=0.5), method=method)
length(unique(unlist(lapply(multifit, get_ranPars, which="lambda")))) # 3
## Fitting the same variance for all binomial responses:
multifit <- fitme(cbind(npos,nneg)~1+Matern(1|x+y),data=genoInSpace,</pre>
                  family=multi(responses=c("type1","type2")),
                  init=list(lambda=NA), # forcing 'outer' estimation for fitme
                  fixed=list(rho=1,nu=0.5), method=method)
length(unique(unlist(lapply(multifit, get_ranPars, which="lambda")))) # 1
multifit <-
 corrHLfit(cbind(npos,nneg)~1+Matern(1|x+y),data=genoInSpace,
            family=multi(responses=c("type1","type2")),
            init.corrHLfit=list(lambda=1), # forcing 'outer' estimation for corrHLfit
            ranFix=list(rho=1,nu=0.5), method=method)
```

```
length(unique(unlist(lapply(multifit, get_ranPars, which="lambda")))) # 1
}
```

mν

Virtual factor for multivariate responses

## **Description**

**Motivation**: In a multivariate-response model fitted by fitmv, one may wish to fit a random-coefficient term appearing in *s* submodels, that is a random effect with realized values for each of these submodels and each group, with values possibly correlated among submodels within groups. Hence one might wish to specify it as a term of the form (<submodel>|group), where <submodel> would represent a factor for the *s* submodels. But the data are not expected to contain a factor for these submodels, so such a syntax would not work without substantial data reshaping. Instead, this effect can be stated as mv(...) where the ... are the indices of the submodels here the random effect appears. For example if submodels 2 and 3 include this random-coefficient term, the term can be specified as (mv(2,3)|group).

Composite random effects, as defined in spaMM-package and illustrated by a bivariate-response quantitative-genetic model (Examples in Gryphon), combine correlations among response variables of different submodels as specified by mv(), and correlations within each response variable(as specified by a relatedness matrix in the same example).

The mv(...) expression is treated as a factor for all purposes, meaning or example that (0+mv(2,3)|group) can also be used, leading (as for any factor) to an alternative parametrization of the same random-coefficient model (see Examples). The parametrization through (0+mv...) is generally recommended as its results are easier to interpret. The random-effect term is treated as a random-coefficient term for all purposes, meaning for example that fixed values can be specified for its parameters using the ranCoefs syntax (see Examples).

## Usage

```
# mv(...)
```

## Arguments

... Indices of all the submodels (possibly more than two) where the random effect involving this virtual factor appears.

### Value

Not a function, hence no return value. In the summary of the fit, levels for the different submodels s within each group are labelled .mvs.

#### See Also

Gryphon for example of composite random effects.

The X2X argument of fitmv for fixed effects shared across sub-models.

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### **Examples**

```
if (spaMM.getOption("example_maxtime")>1.1) {
## data preparation
data("wafers")
me <- fitme(y ~ 1+(1|batch), family=Gamma(log), data=wafers, fixed=list(lambda=0.2))</pre>
set.seed(123)
wafers$y1 <- simulate(me, type="marginal")</pre>
wafers$y2 <- simulate(me, type="marginal")</pre>
## fits
(fitmv1 <- fitmv(</pre>
 submodels=list(mod1=list(formula=y1~X1+(mv(1,2)|batch), family=Gamma(log)),
                 mod2=list(formula=y2~X1+(mv(1,2)|batch), family=Gamma(log))),
 data=wafers))
# alternative '0+' parametrization of the same model:
(fitmv2 <- fitmv(</pre>
 submodels=list(mod1=list(formula=y1~X1+(0+mv(1,2)|batch), family=Gamma(log)),
                 mod2=list(formula=y2~X1+(0+mv(1,2)|batch), family=Gamma(log))),
 data=wafers))
# relationship between the *correlated* effects of the two fits
ranef(fitmv2)[[1]][,2]-rowSums(ranef(fitmv1)[[1]]) # \sim 0
# fit with given correlation parameter:
update(fitmv2, fixed=list(ranCoefs=list("1"=c(NA,-0.5,NA))))
}
```

negbin

Family function for negative binomial "2" response (including truncated variant).

#### **Description**

Returns a GLM family object for negative-binomial model with variance quadratically related to the mean  $\mu$ : variance= $\mu + \mu^2$ /shape, where the shape parameter need or need not be specified, depending on usage. The zero-truncated variant can be specified as negbin2(., trunc = 0L). See negbin1 for the alternative negative-binomial model with variance "linearly" related to the mean.

A **fixed-effect** residual-dispersion model can be fitted, using the resid.model argument, which is used to specify the form of the logarithm of the shape parameter. Thus the variance of the response become  $\mu + \mu^2/\exp(<\operatorname{specified linear expression}>)$ .

negbin(.) is an alias for negbin2(.) (truncated or not), and Tnegbin(.) is an alias for negbin2(., trunc = 0L).

#### Usage

```
# (the shape parameter is actually not requested unless this is used in a glm() call)
#
negbin2(shape = stop("negbin2's 'shape' must be specified"), link = "log", trunc = -1L,
```

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Tnegbin(shape = stop("Tnegbin's 'shape' must be specified"), link = "log")

```
LLgeneric = TRUE)
# For use with glm(), both negbin2's 'shape' and glm's method="llm.fit" are needed.
# alias with distinct arguments:
```

## **Arguments**

shape	Shape parameter of the underlying Gamma distribution: the present negative binomial distribution can be represented as a Poisson-Gamma mixture, where the conditional Poisson mean is $\mu$ times a Gamma random variable with mean 1 and variance 1/shape (as produced by rgamma(., shape=shape, scale=1/shape)).
link	log, sqrt or identity link, specified by any of the available ways for GLM links (name, character string, one-element character vector, or object of class link-glm as returned by make.link).
trunc	Either 0L for zero-truncated distribution, or -1L for default untruncated distribution.
LLgeneric	For development purposes, not documented.

### **Details**

shape is the k parameter of McCullagh and Nelder (1989, p.373) and the theta parameter of Venables and Ripley (2002, section 7.4). The latent Gamma variable has mean 1 and variance 1/shape.

The name NB\_shape should be used to set values of shape in optimization control arguments of the fitting functions (e.g., fitme(.,init=list(NB\_shape=1))); but fixed values are set by the shape argument.

The returned family object is formally suitable for usage with glm if the shape argument is specified, but such usage is *not* recommended as it will lead to incorrect results for the zero-truncated case.

# Value

A family object with structure similar to stats:: family object but with additional member functions for usage with **spaMM** fitting functions.

#### References

McCullagh, P. and Nelder, J.A. (1989) Generalized Linear Models, 2nd edition. London: Chapman & Hall.

Venables, W. N. and Ripley, B. D. (2002) Modern Applied Statistics with S-PLUS. Fourth Edition. Springer.

```
## Fitting negative binomial model with estimated scale parameter:
data("scotlip")
fitme(cases~I(prop.ag/10)+offset(log(expec)),family=negbin(), data=scotlip)
```

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```
\label{log-expec} negfit <- fitme(I(1+cases)^I(prop.ag/10)+offset(log(expec)), family=Tnegbin(), data=scotlip) \\ simulate(negfit,nsim=3)
```

negbin1

Alternative negative-binomial family

## **Description**

Returns a family object suitable as a fitme argument for fitting negative-binomial models with variance linearly (affinely) related to the mean  $\mu$ : variance= $\mu + \mu$ /shape, where the shape parameter need or need not be specified, depending on usage. The model described by such a family is characterized by a linear predictor, a link function, and such a negative-binomial model for the residual variation. The zero-truncated variant of this family is also handled.

A **fixed-effect** residual-dispersion model can be fitted, using the resid.model argument, which is used to specify the form of the logarithm of the shape parameter. Thus the variance of the response become  $\mu + \mu/\exp(<\operatorname{specified linear expression}>)$ .

## Usage

```
negbin1(shape = stop("negbin1's 'shape' must be specified"), link = "log", trunc = -1L)
```

### **Arguments**

shape	Parameter controlling the mean-variance relationship of the negbin1 distribution. This distribution can be represented as a Poisson-Gamma mixture, where the conditional Poisson mean is $\mu$ times a Gamma random variable with mean 1 and variance $1/(\text{shape}*\mu)$ as produced by rgamma(., shape=sh,scale=1/sh) where sh=shape* $\mu$ , meaning that the family shape parameter controls, but differs from, the gamma shape parameter.
link	log, sqrt or identity link, specified by any of the available ways for GLM links (name, character string, one-element character vector, or object of class link-glm as returned by make.link).
trunc	Either 0L for zero-truncated distribution, or -1L for default untruncated distribution.

## **Details**

The name NB\_shape should be used to set values of shape in optimization control arguments of the fitting functions (e.g., fitme(.,init=list(NB\_shape=1))); but fixed values are set by the shape argument.

The family should not be used as a glm argument as the results would not be correct.

## Value

A list, formally of class c("LLF", "family"). See LL-family for details about the structure and usage of such objects.

numInfo

### See Also

Examples in LL-family. resid.model for an example with a residual-dispersion model.

numInfo	Information matrix		
---------	--------------------	--	--

## **Description**

Computes by numerical derivation the observed information matrix for (ideally) all parameters for mean response model, that is, the matrix of second derivatives of negative log likelihood. The default value of the which argument shows all classes of parameters that should be handled, including random-effect parameters (lambda, ranCoefs, corrPars, and hyper), residual dispersion parameters (phi, NB\_shape for negbin1 and negbin2, and beta\_prec for beta\_resp and betabin), and fixed-effect coefficients (beta).

Model fits including a phi-resid.model are not fully handled, in two ways: the information matrix does not include their parameters; and if the residual dispersion model include random effects, there is good reason for the numInfo calculation to detect that the fit has not maximized marginal likelihood with respect to most parameters.

## Usage

#### **Arguments**

Fit object returned by a <b>spaMM</b> fitting function.
Whether to perform internal computations on a transformed scale (but computation on transformed scale may be implemented for fewer classes of models than default computation).
NULL, or character vector giving the sets of parameters with respect to which derivatives are to be computed. The NULL default is equivalent to c("lambda", "ranCoefs", "corrPars", "hyper", "phi", "NB_shape", "beta_prec", "beta") for ML fits, and to the same except "beta" (fixed effects) for REML fits.
Boolean; whether to perform some checks for possible problems (see Details).
numeric value, or FALSE; if it is a nonzero numeric value, eigenvalues of the matrix are checked and values smaller than sing are highlighted in output (see Value). This will highlight nearly-singular information matrices, but also those with large negative eigenvalues.
Boolean: whether to print (as a list) the estimates of the parameters for which the Hessian will be computed, additional information about possibly ignored parameters, possible misuse of REML fits, and a (sort of) progress bar if the procedure is expected to last more than a few seconds.

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list of arguments; its name anticipates that it might allow hazardous manipulations in a later version of **spaMM**. But currently only the innocuous element verbose of the list will be taken into account. Notably, refit\_hacks=list(verbose=c(TRACE=TRUE)) can be used to give information on parameter values used in the computation of numerical derivatives.

.. Arguments passed to numDeriv::hessian and numDeriv::grad.

#### **Details**

The computation of a second derivatives is not necessarily meaningful if a first derivative does not vanish at the parameter estimates. This may occur in particular when the objective function (say, marginal likelihood) is maximized at a boundary of the parameter space (say, at zero for lambda estimates). Further, for such values at a boundary, only one-sided derivatives can be computed, and this is not handled by numDeriv::hessian. So, some checks may be requested to detect nonzero gradients and parameters estimated at their boundaries. The boundary checks are currently performed for lambda and ranCoefs estimates, if check\_deriv is set to TRUE or to NULL. Other parameters are not (yet) checked, so numInfo may sometimes fails when such other parameter estimates are at a boundary. If check\_deriv is set to TRUE, an additional systematic check of the gradient with respect to all target parameters is performed.

#### Value

NULL or a matrix.

NULL is returned if no parameter is found with respect to which a numerical information "should" be computed (where what should be done depends on the which and check\_derivs arguments).

Otherwise a matrix is returned, with an eigvals attribute if sing was non-zero. This attribute is a numeric vector of eigenvalues of the matrix. If some eigenvalue(s) were lower than sing, the vector has additional class "singeigs" so that its printing is controlled by an ad-hoc print.singeigs method highlighting the small eigenvalues.

```
data("wafers")
lmmfit <- fitme(y ~X1+X2+X1*X3+X2*X3+I(X2^2)+(1|batch),data=wafers)
numinfo <- numInfo(lmmfit)
(SEs <- sqrt(diag(solve(numinfo))))
#
# => beta SEs here equal to conditional SEs shown by fit summary.
# Other SEs can be compared to the approximate ones
# for log(phi) and log(lambda), given by
#
# update(lmmfit, control=list(refit=TRUE))
#
# => 1118*0.5289 and 10840*0.1024

data("blackcap")
maternfit <- fitme(migStatus ~ means+ Matern(1|longitude+latitude),data=blackcap)
numInfo(maternfit)</pre>
```

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options

spaMM options settings

## **Description**

Allow the user to set and examine a variety of *options* which affect operations of the spaMM package.

### Usage

```
spaMM.options(..., warn = TRUE)
spaMM.getOption(x)
```

## **Arguments**

Χ

a character string holding an option name.

warn

Boolean: whether to warn if a previously undefined options is being defined (a protection against typos).

. . .

A named value or a list of named values. The following values, with their defaults, are used in spaMM:

LevenbergM=NULL: NULL or boolean. Whether to use a Levenberg-Marquardt-like algorithm (see Details) by default in most computations. But it is advised to use instead control.HLfit=list(LevenbergM=...) to control this on a case-by-case basis. The joint default behaviour is that Levenberg-Marquardt is used by default for binomial response data that takes only extreme values (in particular, for binary 0/1 response), and that for other models the fitting algorithm switches to it if divergence is suspected. FALSE inhibits its use; TRUE forces its use for all iterative least-square fits, except when 'confint()' is called.

example\_maxtime=0.7: Used in the documentation and tests to control whether the longer examples should be run. The approximate running time of given examples on one author's laptop is compared to this value.

optimizer1D="optimize": Optimizer for one-dimensional optimization. If you want to control the initial value, you should select another optimizer.

optimizer=".safe\_opt": Optimizer for optimization in several dimensions. Use optimizer="nloptr" to call nloptr with method "NLOPT\_LN\_BOBYQA"; use optimizer="bobyqa" to call bobyqa; and use optimizer="L-BFGS-B" to call optim with method "L-BFGS-B". The default ".safe\_opt" uses nloptr except in some cases where it expects or detects problems with it (the source code should be consulted for details). The optimizer can also be specified on a fit-by-fit basis as the value of control\$optimizer in a fitme call, or as the value of control.corrHLfit\$optimizer.

nloptr: Default control values of nloptr calls.

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- bobyqa: Default control values of bobyqa calls.
- maxLambda=1e10: The maximum value of lambda: higher fitted lambda values in HLfit are reduced to this. Since version 3.1.0, a much smaller lambda bound is deduced from maxLambda for COMPoisson and log-link response families.
- regul\_lev\_lambda Numeric (default: 1e-8); lambda leverages numerically 1 are replaced by 1- regul\_lev\_lambda
- COMP\_maxn: Number of terms for truncation of infinite sums that are evaluated in the fitting of COMPoisson models.
- CMP\_asympto\_cond: Function returning the condition for applying an approximation or the COMPoisson response family, as detailed in COMPoisson.
- Gamma\_min\_y=1e-10: A minimum response value in Gamma-response models; used to check data, and in simulate() to correct the simulation results.
- QRmethod: A character string, to control whether dense matrix or sparse matrix methods are used in intensive matrix computations, overcoming the default choices made by spaMM in this respect. Possible values are "dense" and "sparse".
- matrix\_method: A character string, to control the factorization of dense model matrices. Default value is "def\_sXaug\_EigenDense\_QRP\_scaled". The source code should be consulted for further information.
- Matrix\_method: A character string, to control the factorization of sparse model matrices. Default value is "def\_sXaug\_Matrix\_QRP\_CHM\_scaled". The source code should be consulted for further information.
- stylefns: Default colors of some screen output (notably that of some fitting functions when called with argument verbose=c(TRACE=TRUE))
- barstyle: Integer, or Boolean interpreted as Integer, or quoted expression evaluating to such types; controlling the display of some progress bars. If zero, no progress bar should be displayed; otherwise, a bar should be displayed. Further, when txtProgressBar is called, barstyle is passed as its style argument. Default is quote(if(interactive()) {3L} else {0L}) (in a parallel setting, child processes may display the bar if the parent process is interactive).

and many other undocumented values for programming or development purposes. Additional options without default values can also be used (e.g., see algebra).

## **Details**

spaMM.options() provides an interface for changing maximal values of parameters of the Matérn correlation function. However, it is not recommended to change these values unless a spaMM message specifically suggests so.

By default spaMM use Iteratively Reweighted Least Squares (IRLS) methods to estimate fixed-effect parameters (jointly with predictions of random effects). However, a Levenberg-Marquardt algorithm, as described by Nocedal & Wright (1999, p. 266), is also implemented. The Levenberg-Marquardt algorithm is designed to optimize a single objective function with respect to all its parameters. It is thus well suited to compute a PQL fit, which is based on maximization of a single function, the h-likelihood. By contrast, in a fit of a mixed model by (RE)ML, one computes jointly

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fixed-effect estimates that maximizes marginal likelihood, and random-effect values that maximize h-likelihood given the fixed-effect estimates. The gradient of marginal likelihood with respect to fixed-effect coefficients does not generally vanishes at the solution (although it remains close to zero except in "difficult" cases with typically little information in the data). The Levenberg-Marquardt algorithm is not directly applicable in this case, as it may produce random-effect values that increases marginal likelihood rather than h-likelihood. The (RE)ML variant of the algorithm implemented in spaMM may therefore use additional nested h-likelihood-maximizing steps for correcting random-effect values. In version 3.1.0 this variant was revised for improved performance in difficult cases.

#### Value

For spaMM.getOption, the current value set for option x, or NULL if the option is unset.

For spaMM.options(), a list of all set options. For spaMM.options(<name>), a list of length one containing the set value, or NULL if it is unset. For uses setting one or more options, a list with the previous values of the options changed (returned invisibly).

#### References

Jorge Nocedal and Stephen J. Wright (1999) Numerical Optimization. Springer-Verlag, New York.

## **Examples**

```
spaMM.options()
spaMM.getOption("example_maxtime")
## Not run:
spaMM.options(maxLambda=1e06)
## End(Not run)
```

pedigree

Fit mixed-effects models incorporating pedigrees

## Description

This example illustrates how to use spaMM for quantitative genetic analyses. spaMM appears competitive in terms of speed for GLMMs with large data sets, particularly when using the PQL method, which may be a quite good approximation in such cases. For large pedigrees it may be useful to compute the inverse of the relationship matrix using some efficient ad hoc algorithm, then to provide it as argument of the fit using the covStruct(list(precision=...)) syntax. If the precision matrix is not specified, spaMM will generally evaluate it to assess whether it should use sparse-precision methods. see sparse\_precision for further control of this computation, on another example from quantitative genetics.

#### See Also

```
sparse_precision
```

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### **Examples**

```
## Not run:
# if(requireNamespace("pedigreemm", quietly=TRUE)) {
    ## derived from help("pedigreemm")
    # p1 <- new("pedigree",</pre>
               sire = as.integer(c(NA,NA,1, 1,4,5)),
               dam = as.integer(c(NA,NA,2,NA,3,2)),
              label = as.character(1:6))
    # A <- pedigreemm::getA(p1) ## relationship matrix
# }
## => Manually-built matrix:
A <- matrix(NA, ncol=6,nrow=6)
A[lower.tri(A,diag=TRUE)] < -c(8,0,4,4,4,2,8,4,0,2,5,8,2,5,4.5,8,5,2.5,9,5.5,9)/8
A <- Matrix::forceSymmetric(A,uplo = "L")
colnames(A) \leftarrow rownames(A) \leftarrow 1:6
## data simulation
cholA <- chol(A)</pre>
varU <- 0.4; varE <- 0.6; rep <- 20
n <- rep*6
set.seed(108)
bStar <- rnorm(6, sd=sqrt(varU))
b <- crossprod(as.matrix(cholA),bStar)</pre>
ID <- rep(1:6, each=rep)</pre>
e0 <- rnorm(n, sd=sqrt(varE))</pre>
y \leftarrow b[ID]+e0
obs <- data.frame(y=y,IDgen=ID,IDenv=ID) ## two copies of ID for readability of GLMM results
fitme(y ~ 1+ corrMatrix(1|IDgen) , corrMatrix=A,data=obs,method="REML")
obs$y01 <- ifelse(y<1.3,0,1)
fitme(y01 ~ 1+ corrMatrix(1|IDgen)+(1|IDenv), corrMatrix=A,data=obs,
      family=binomial(), method="REML")
prec_mat <- solve(A)</pre>
colnames(prec_mat) <- rownames(prec_mat) <- rownames(A) # important</pre>
fitme(y01 ~ 1+ corrMatrix(1|IDgen)+(1|IDenv) , covStruct=list(precision=prec_mat),
      data=obs, family=binomial(), method="REML")
## End(Not run)
```

phi-resid.model

Residual dispersion model for gaussian and Gamma response

## **Description**

A model can be specified for the residual-dispersion parameter  $\phi$  of gaussian and Gamma response families. This model may or may not include random effects. The resid.model argument of all fitting functions is used to specify this model and to control its fit. resid.model is **either** a

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formula (without left-hand side) for the dispersion parameter phi of the residual error (a log link is assumed); **or** a list of arguments similar to those of a standard fitme call.

The residual-dispersion model is fitted by a specific method (see Details) involving estimation of its parameters by the fit of a Gamma-response model to response values computed by the parent fitting function (i.e., the fitting function called to fit the joint models for main response and for residual dispersion). For mixed-effect residual-dispersion models, the fitme function is used internally to fit this Gamma-response model (irrespective of the parent fitting function used, which may not be fitme).

## Usage

```
# 'resid.model' argument of fitting functions (fitme(), HLfit(), etc)
```

### **Arguments**

If resid.model is a list, it must include a formula element (model formula without left-hand side, as when resid.model is only a formula). The following additional arguments may be useful:

family	The family is always Gamma. The default link is log. The identity link can be tried but may fail because only the log link ensures that the fitted $\phi$ is positive.
fixed	fixed values of parameters of the residual dispersion model itself. Same usage as documented in fitme, except that it is better not to try to fix its phi (see Details).
etaFix	To fix some of the fixed-effect coefficients, as in the mean response, and with the same format. Note that the same effect can usually be acheived by an offset in the formula.
control.dist	A list of arguments that control the computation of the distance argument of the correlation functions. Same usage as documented in HLCor
rand.family	A family object or a list of family objects describing the distribution of the random effect(s). Same usage as documented for $HLfit$
init, lower, upper, control	
	with same usage as documented in $\ensuremath{\mbox{fitme}}.$ These arguments may (partly) be ignored in some cases.

Other arguments should be ignored (see Details).

### **Details**

The following elements should not be specified in resid.model, for the specified reasons:

**method** which is constrained to be identical to the method from the parent call;

**control.HLfit, control.glm** constrained to be identical to the same-named controls from the parent call;

**resid.model** constrained: no resid.model for a resid.model;

the phi of the Gamma family of the residual dispersion model This parameter is by default set to 1, in agreement with the theory underlying the estimation procedure for the residual model; it can be set to another value, and a resid.model's fixed=list(phi=NA) will even force its estimation, but this is not warranted;

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### **REMLformula** constrained to NULL;

data The data of the parent call are used, so they must include all the variables required for the resid.model;

prior.weights constrained: no prior weights;

**verbose** constrained: use the verbose argument of the fitting function instead to control a progress line summarizing the results of the resid.model fit at each iteration of main loop of the parent call (see the next section of the Details).

**init.HLfit** if used, this argument may affect the fits. However, it is best ignored in practice: users would have hard time guessing good initial values, and bad ones might have unwarranted effects.

**Progress reports of the fitting procedure:** Fits with a mixed-effect residual-dispersion model involve repeated "nested" fits of the latter model (each of them itself tipycally involving "double-nested" fits of a mixed-effect model with fixed random-effect parameters). This can be slow particularly when the residual-dispersion model involve spatial effects. A specific element phifit of the verbose vector controls screen information about progress of such fits during the full-model fit: when set to 0 (or FALSE) there is no report. For higher values a one-line message is output at the end of each "nested" call, but it may be overwritten by the next one-line message. So the ultimately visible output depends on control of overwriting. When verbose["phifit"] is set to 1 (or TRUE) each output overwrites the previous one so the ultimately visible output is from the last "nested" call; when it is set to 2, the final line of output of each "nested" call remains visible; when set to 3, a line of output remains visible from each "double-nested" call.

**Methods:** The present implementation of the Gamma-response procedure used to fit (fixed-effect) residual dispersion models is based on its exact components as detailed by Smyth et al. 2001. **spaMM** also implements an ML version of this REML procedure (where the leverage corrections used in the REML procedure are set to zero). Smyth et al. discuss more approximate versions of the components, considered in the early h-likelihood literature and elsewhere.

Lee and Nelder (2006) extend the REML procedure to mixed-effects residual dispersion models. Again, **spaMM** also implements ML and REML versions of these procedures (using distinct "standardizing" leverages as detailed in hatvalues.HLfit), and additionally use by default the full Laplace approximation (with observed Hessian) for fitting the Gamma-response mixed-effect model, instead of the approximation using expected Hessian considered in the h-likelihood literature.

When the residual-dispersion model includes random effects, no single likelihood objective function appears to be maximized by the joint fit of mean-response and residual dispersion models. A procedure such as numInfo may then detect that the likelihood gradient does not vanish for all parameters. Indeed, this limitation is "relatively obvious" in original formulations relying on both marginal likelihood and restricted likelihood concepts to fit different parameters of the joint model. But this limitation is also true in the case where marginal likelihood (actually, its Laplace approximation, although the issue could persist even if exact Gamma-GLMM likelihood were used) is used in the residual-dispersion fit.

#### Value

When such dispersion models are fitted, the resulting fits are embedded in the main fit object. The get\_fittedPars extractor will by default )as controlled by its argument phiPars) include in its return value the rdisPars element, which is the list of parameters of the residual-dispersion fit,

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in the same format as a get\_fittedPars value for the mean-response model (rdisPars may also include fits of other residual-dispersion models described in resid.model). The phi element of the get\_fittedPars value will further contain the residual-dispersion fit itself, as a "glm" or, when it includes random effects, as a "HLfit" object.

#### References

Lee, Y. and Nelder, J.A. (2006), Double hierarchical generalized linear models (with discussion). Journal of the Royal Statistical Society: Series C (Applied Statistics), 55: 139-185. doi:10.1111/j.14679876.2006.00538.x

Lee, Y., Nelder, J. A. and Pawitan, Y. (2006) Generalized linear models with random effects: unified analysis via h-likelihood. Chapman & Hall: London.

Smyth, G. K., Huele, F., and Verbyla, A. P. 2001. Exact and approximate REML for heteroscedastic regression, Stat. Modelling 1, 161–175.

## **Examples**

plot.HLfit

Model checking plots for mixed models

### **Description**

This function provides diagnostic plots for residual errors from the mean model and for random effects. Plots for the mean models are similar to those for GLMs. They use *standardized* deviance residuals as described by Lee et al. (2006, p.52). This means that plots for residual errors use the residuals provided by residuals(<fit object>, type="std\_dev\_res"); and that plots for random effects likewise consider standardized values.

### **Usage**

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### **Arguments**

X	An object of class HLfit, as returned by the fitting functions in spaMM.
which	A vector of keywords for different types of plots. By default, two types of plots are presented on different devices: diagnostic plots for mean values, and diagnostic plots for random effects. Either one can be selected using this argument. Use keyword "predict" for a plot of predicted response against actual response.
titles	A list of the main (inner and outer) titles of the plots. See the default value for the format.
control	A list of default options for the plots. Defaults are pch="+" and pcol="blue" for points, and lcol="red" for curves.
ask	Logical; passed to devAskNewPage which is run when a new device is opened by code.HLfit.
	Options passed from plot. HLfit to par.

## **Details**

In principle the standardized deviance residuals for the mean model should have a nearly Gaussian distribution hence form a nearly straight line on a Q-Q plot. However this is (trivially) not so for well-specified (nearly-)binary response data nor even for well-specified Poisson response data with moderate expectations. Hence this plot is not so useful. The DHARMa package proposes betterbehaved diagnostic plots (but the p-value that appears on one of these plots may not stand for a valid goodness-of-fit test). The current version of DHARMa should handle spaMM fit objects; otherwise, see https://github.com/florianhartig/DHARMa/issues/95 for how to run DHARMa procedures on spaMM output.

## Value

Returns the input object invisibly.

#### References

Lee, Y., Nelder, J. A. and Pawitan, Y. (2006). Generalized linear models with random effects: unified analysis via h-likelihood. Chapman & Hall: London.

plot\_effects

plot\_effects

Partial-dependence effects and plots

## **Description**

The function pdep\_effects evaluates, and the function plot\_effects plots, *partial-dependence* effects.

pdep\_effects evaluates the effect of a given fixed-effect variable, as (by default, the average of) predicted values on the response scale, over the empirical distribution of all other fixed-effect variables in the data, and of inferred random effects. This can be seen as the result of an experiment where specific treatments (given values of the focal variable) are applied over all conditions defined by the other fixed effects and by the inferred random effects. Thus, apparent dependencies induced by associations between predictor variables are avoided (see Friedman, 2001, from which the name "partial dependence plot" is taken; or Hastie et al., 2009, Section 10.13.2). This also avoids biases of possible alternative ways of plotting effects. In particular, such biases occur if the response link is not identity, and if averaging is performed on the linear-predictor scale or when other variables are set to some conventional value other than its average.

pdep\_effects also compute intervals of the type defined by its intervals argument (by default, prediction intervals) and of nominal coverage defined by the level argument (it may make particular sense to choose a level<0.95 to better visualize effects). By default, it returns a data frame of average values of point predictions and interval bounds for each value of the focal variable (so the intervals may briefly be described as mean prediction intervals, for want of better), but it can also return lists of all predictions.

A plot function is available for numeric or factor predictors: plot\_effects calls pdep\_effects and produces a simple plot (using only base graphic functions) of its results, including prediction bands representing the two average one-sided widths of intervals. The last section of the Examples shows how to obtain more elaborate plots including the same information using **ggplot2**.

If added to the plot, the raw data may appear to depart from the partial-dependence predictions, since the data are a priori affected by the associations between variables which the predictions free themselves from. An adapted plot of fit residuals may be then be more useful, and the Examples also show how it can be performed.

#### **Usage**

## **Arguments**

object

An object of class HLfit, as returned by the fitting functions in spaMM.

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Character string: the name of the predictor variable whose effect is to be repre-

sented. The variable must be numeric for plot\_effects but not necessarily so for pdep\_effects. newdata If non-NULL, a data frame passed to predict. HLfit, whose documentation should be consulted for further details. effects If non-NULL, a data frame to substitute to the one produced by default by pdep\_effects. xlab If non-NULL, a character string: X-axis label for the plot. ylab If non-NULL, a character string: Y-axis label for the plot. ylim The plot's ylim argument. Default is based on the (0.025,0.975) quantiles of the response. Color control arguments, in the format produced by col2rgb. rgb.args add Boolean: whether to add graphic elements of a previous plot produced by plot\_effects Integer: for a numeric predictor variable, this controls the number of values at length.out which predictions are evaluated. By default, predictions are made at regular intervals over the range of the predictor variable. If length.out=0, predictions are made for the actual values of the focal predictor in the data. The default behaviour is also overriden by using focal\_values, in which case predictions are evaluated at the given focal\_values (as if length.out=0), unless a nonzero length.out is also specified. In the latter case, predictions are evaluated at regular intervals over the range of focal\_values. intervals, level Passed to predict. HLfit, whose documentation should be consulted for further details.

focal\_values, levels

focal\_var

focal\_values may be used to specify the values of the focal variable at which predictions are evaluated. For factor variables, levels is an older implementation of this control and is now redundant.

tion of this control, and is now redundant.

indiv Boolean: whether to return all predictions given the values of other predictors

in the newdata, or only their means.

... Further arguments passed by plot\_effects to pdep\_effects, or by pdep\_effects

to predict.HLfit.

## Value

For pdep\_effects, a nested list, or a data frame storing values of the focal\_var, average point predictions pointp and bounds low and up of intervals, depending on the indiv argument. When indiv is TRUE, each sublist contains vectors for pointp, low and up.

For plot\_effects, the same value, returned invisibly.

### References

- J.H. Friedman (2001). Greedy Function Approximation: A Gradient Boosting Machine. Annals of Statistics 29(5):1189-1232.
- J. Friedman, T. Hastie and R. Tibshirani (2009) The Elements of Statistical Learning, 2nd ed. Springer.

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```
data("scotlip")
hlcor <- HLCor(cases~I(prop.ag/10) +adjacency(1|gridcode)+offset(log(expec)),
           adjMatrix=Nmatrix,family=poisson(),data=scotlip)
plot_effects(hlcor,focal_var="prop.ag",ylim=c(0,max(scotlip$cases)))
points(cases~prop.ag, data=scotlip, col="blue",pch=20)
# Impose specific values of a numeric predictor using 'focal_values':
plot_effects(hlcor, focal_var="prop.ag", focal_values=1:5)
### Adding 'partial residuals' [residuals relative to predict(<fit object>),
### but plotted relative to pdep_effects() predictions]:
# One first needs predictions for actual values of the predictor variable,
# provided by pdep_effects(.,length.out=0L):
pdep_points <- pdep_effects(hlcor,focal_var="prop.ag",length.out=0L)</pre>
# Rename for easy prediction for each observation, and add the residuals
# of the actual fit, using the default residuals() i.e. deviance ones:
rownames(pdep_points) <- pdep_points$focal_var</pre>
pdep_res <- pdep_points[paste(hlcor$data$prop.ag), "pointp"] +</pre>
              residuals(hlcor)
points(x = hlcor$data$prop.ag, y = pdep_res, col = "red", pch = 20)
## Not run:
## Plotting pdep-effects for different categories, using ggplot.
library(ggplot2)
data("Gryphon")
tmp <- na.omit(Gryphon_df)</pre>
spfit <- spaMM::fitme(TARSUS ~ BWT*sex, data = tmp)</pre>
tmp$sex <- "1"
pdep_1 <- pdep_effects(spfit,"BWT", newdata=tmp, level=qnorm(0.75))</pre>
                    qnorm(0.75) to get the so-called 'probable error'.
tmp$sex <- "2"
pdep_2 <- pdep_effects(spfit,"BWT", newdata=tmp, level=qnorm(0.75))</pre>
pdep_1$sex <- "1" ; pdep_2$sex <- "2"
pdep <- rbind(pdep_1,pdep_2)</pre>
ggplot(pdep,aes(y = pointp , x = focal_var ,col = sex, fill=sex)) + geom_point() +
  geom_ribbon(aes(ymin = low, ymax = up), alpha = 0.3) + xlab("BWT") +
  ylab("TARSUS")
## End(Not run)
```

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Poisson	Family function for GLMs and mixed models with Poisson and zero-truncated Poisson response.

## **Description**

Poisson (with a capital P) is a family that specifies the information required to fit a Poisson generalized linear model. Differs from the base version stats::poisson only in that it handles the zero-truncated variant, which can be specified either as Tpoisson(<link>) or as Poisson(<link>, trunc = 0L). The truncated poisson with mean  $\mu_T$  is defined from the un-truncated poisson with mean  $\mu_U$ , by restricting its response strictly positive value.  $\mu_T = \mu_U/(1-p0)$ , where  $p0 := \exp(-\mu_U)$  is the probability that the response is 0.

## Usage

```
Poisson(link = "log", trunc = -1L, LLgeneric=TRUE)
Tpoisson(link="log")
# <Poisson object>$linkfun(mu, mu_truncated = FALSE)
# <Poisson object>$linkinv(eta, mu_truncated = FALSE)
```

#### **Arguments**

link	log, sqrt or identity link, specified by any of the available ways for GLM links (name, character string, one-element character vector, or object of class link-glm as returned by make.link).
trunc	Either $\theta L$ for zero-truncated distribution, or $\neg 1L$ for default untruncated distribution.
eta, mu	Numeric (scalar or array). The linear predictor; and the expectation of response, truncated or not depending on mu_truncated argument.
mu_truncated	Boolean. For linkinv, whether to return the expectation of truncated $(\mu_T)$ or un-truncated $(\mu_U)$ response. For linkfun, whether the mu argument is $\mu_T$ , or is $\mu_U$ but has $\mu_T$ as attribute $(\mu_U)$ without the attribute is not sufficient).
LLgeneric	For development purposes, not documented.

# Details

Molas & Lesaffre (2010) developed expressions for deviance residuals for the truncated Poisson distribution, which were the ones implemented in **spaMM** until version 3.12.0. Later versions implement the (non-equivalent) definition as "2\*(saturated\_logLik - logLik)".

predict, when applied on an object with a truncated-response family, by default returns  $\mu_T$ . The simplest way to predict  $\mu_U$  is to get the linear predictor value by predict(.,type="link"), and deduce  $\mu_U$  using linkinv(.) (with default argument mu\_truncated=FALSE), since getting  $\mu_U$  from  $\mu_T$  is comparatively less straightforward. The mu.eta member function is that of the base poisson family, hence its mu argument represents  $\mu_U$ .

simulate, when applied on an object with a truncated-response family, simulates the truncated family. There is currently no clean way to override this (trying to passtype="link" to predict will not have the intended effect).

post-fit

#### Value

A family object suitable for use with glm, as stats:: family objects.

#### References

McCullagh, P. and Nelder, J.A. (1989) Generalized Linear Models, 2nd edition. London: Chapman & Hall.

Molas M. and Lesaffre E. (2010). Hurdle models for multilevel zero-inflated data via h-likelihood. Statistics in Medicine 29: 3294-3310.

## **Examples**

post-fit

Applying post-fit procedures on spaMM results

## **Description**

Packages implementing post-fit procedures define helper functions which may not handle **spaMM**'s fit objects, or which have not always handled them, or which can handle them correctly only with some non-default arguments. This documentation topic gives further directions to apply some such post-fit procedures (from packages **DHARMa**, **RLRsim**, **multcomp** and **lmerTest**) to these fit objects.

For other procedures not considered here, diagnosing a failure in a debugging session may suggest a simple solution (as it did for multcomp::glht).

### **Details**

For multiple comparison procedures by multcomp::glht, one has to explicitly give the argument coef.=fixef.HLfit (see Examples; fixef.HLfit is the **spaMM** method for the generic function fixef);

For **DHARMa** plots, see Details of plot. HLfit;

For using **RLRsim::RLRTSim()**, see get\_RLRTSim\_args.

For using **lmerTest::contest()** or **lmerTest::anova()**, see as\_LMLT.

```
if (requireNamespace("multcomp", quietly = TRUE)) {
   library(multcomp)
   set.seed(123)
   irisr <- cbind(iris,id=sample(4,replace=TRUE,size=nrow(iris)))
   irisfit <- fitme(Petal.Length~ Species +(1|id), data=irisr, family=Gamma(log))
   summary(glht(irisfit,mcp("Species" = "Tukey"), coef.=fixef.HLfit))
}</pre>
```

predict

Prediction from a model fit

## Description

The following functions can be used to compute point predictions and/or various measures of uncertainty associated to such predictions:

- \* predict can be used for prediction of the response variable by its expected value obtained as (the inverse link transformation of) the linear predictor  $(\eta)$  and more generally for terms of the form  $\mathbf{X}_n \beta + \mathbf{Z}_n \mathbf{L} \mathbf{v}$ , for new design matrices  $\mathbf{X}_n$  and  $\mathbf{Z}_n$ .
- \* Various components of prediction variances and predictions intervals can also be computed using predict. The get\_... functions are convenient extractors for such components;
- \* get\_predCov\_var\_fix extracts a block of a prediction covariance matrix. It was conceived for the specific purpose of computing the spatial prediction covariances between two "new" sets of geographic locations, without computing the full covariance matrix for both the new locations and the original (fitted) locations. When one of the two sets of new locations is fixed while the other varies, some expensive computations can be performed once for all sets of new locations, and be provided as the fix\_X\_ZAC.object argument. The preprocess\_fix\_corr extractor is designed to compute this argument.

### Usage

```
## S3 method for class 'HLfit'
predict(object, newdata = newX, newX = NULL, re.form = NULL,
                        variances=list(), binding = FALSE, intervals = NULL,
                        level = 0.95, blockSize = 2000L, type = "response",
                        verbose=c(showpbar=eval(spaMM.getOption("barstyle"))),
                    control=list(), na.action=na.omit, cluster_args=list(), ...)
get_predCov_var_fix(object, newdata = NULL, fix_X_ZAC.object, fixdata, re.form = NULL,
                    variances=list(disp=TRUE, residVar=FALSE, cov=FALSE),
                    control=list(), ...)
preprocess_fix_corr(object, fixdata, re.form = NULL,
                   variances=list(residVar=FALSE, cov=FALSE), control=list())
get_fixefVar(...)
get_predVar(..., variances=list(), which="predVar")
get_residVar(...)
get_respVar(...)
get_intervals(..., intervals="predVar")
```

### **Arguments**

object

The return object of fitting functions HLfit,corrHLfit,HLCor... returning an object inheriting from HLfit class.

newdata

Either NULL, a matrix or data frame, or a numeric vector.

If NULL, the original data are reused. Otherwise, all variables required to evaluate model formulas must be included. Which variables are required may depend on

other arguments: see "prediction with given phi's" example, also illustrating the syntax when formulas include an offset.

If newdata is a numeric vector, its names (if any) are ignored. This makes it easier to use predict as an objective function for an optimization procedure such as optim, which calls the objective function on unnamed vectors. However, one must make sure that the order of elements in the vector is the order of first occurrence of the variables in the model formula. This order can be checked in the error message returned when calling predict on a newX vector of clearly wrong size, e.g. predict(<object>, newdata=numeric(0)).

newX

equivalent to newdata, available for back-compatibility

re.form

formula for random effects to include. By default, it is NULL, in which case all random effects are included. If it is NA, no random effect is included. If it is a formula, only the random effects it contains are retained. The other variance components are removed from both point prediction and variances calculations. If you want to retain only the spatial effects in the point prediction, but all variances, either use re.form and add missing variances (on linear predictor scale) manually, or ignore this argument and see Details and Examples for different ways of controlling variances.

variances

A list whose elements control the computation of different estimated variances. predict can return four components of prediction variance: fixefVar, predVar, residVar and respVar, whose definitions is detailed in predVar. They are all returned as attributes of the point predictions.

In particular, variances=list(predVar=TRUE) is suitable for uncertainty in point prediction, distinguished from the response variance given by list(respVar=TRUE). See the predVar help page for further explanations and other options.

intervals

NULL or character string or vector of strings. Provides prediction intervals with nominal level level, deduced from the given prediction variance term, e.g. intervals="predVar". Currently only intervals from fixefVar and predVar (and for LMMs respVar including the residual variance) may have a probabilistic meaning. Intervals returned in other cases are (currently) meaningless.

which

any of "predVar", "respVar", "residVar", "fixefVar", "intervals", or "naive"

level

Coverage of the intervals.

binding

If binding is a character string, the predicted values are bound with the newdata and the result is returned as a data frame. The predicted values column name is the given binding, or a name based on it if the newdata already include a variable with this name. If binding is FALSE, The predicted values are returned as a one-column matrix and the data frame used for prediction is returned as an attribute (unless it was NULL). If binding is NA, a vector is returned, without the previous attributes.

fixdata

A data frame describing reference data whose covariances with variable newdata may be requested.

fix\_X\_ZAC.object

The return value of calling preprocess\_fix\_corr (see trivial Example). This is a more efficient way of providing information about the fixdata for repeated calls to get\_predCov\_var\_fix with variable newdata.

blockSize

For data with many rows, it may be more efficient to perform some operations on slices of the data, and this gives the maximum number or rows of each slice. Further, parallelisation of computations over the slices is possible, as controlled by the cluster\_args argument. Slicing and parallelisation may operate only if covariance matrices are not requested.

type

character string; The returned point predictions are on the response scale if type="response" (the default; for binomial response, a frequency 0<.<1). It is on the linear predictor scale if type="link".

\* The "prediction variance" (as opposed to the response variance, see predVar) that may be returned as a "predVar" attribute of the point predictions is always on the linear predictor scale, even when type="response". If you want to extract this predVar transformed to the response scale, use predict(.,variances=list(respVar=TRUE))

and take the difference between the respVar and residVar attributes of the re-

sult.

\* Prediction intervals (as opposed to the response intervals) will be on the linear predictor or response scale depending on type (new to versions more recent than 3.12.0).

control A list; a warning will direct you to relevant usage when needed.

cluster\_args Passed to makeCluster. Parallel computations are possible if the slicing mech-

anism (as controlled by argument blockSize) is effective.

verbose A vector of booleans; it single currently used element is "showpbar", which

controls whether to show a progress bar in certain prediction variance computa-

tions.

na.action One of the functions dealing with NAs in data frames (see na.omit). if this is

set to na.exclude, NAs will be included in the returned point predictions, for rows of the newdata which do not provide information for all required predictor variables. The effect of the default na.omit is to not include such NAs (this differs from the default of, e.g., predict.lm). Implementation is limited; in particular, na.exclude currently does not have the effect of including NAs in the optional attributes providing (co-)variance information, except the "mv" attribute

for predictions of multivariate-response fits.

... further arguments passed to or from other methods. For the get\_... functions,

they are passed to predict.

#### **Details**

See the predVar help page for information about the different concepts of prediction variances handled by spaMM (uncertainty of point prediction vs. of response) and about options controlling their computation.

If newdata is NULL, predict returns the fitted responses, including random effects, from the object. Otherwise it computes new predictions including random effects as far as possible. For spatial random effects it constructs a correlation matrix  $\mathbf{C}$  between new locations and locations in the original fit. Then it infers the random effects in the new locations as  $\mathbf{C}(\mathbf{L}')^{-1}\mathbf{v}$  (see spaMM for notation). For non-spatial random effects, it checks whether any group (i.e., level of a random effect) in the new data was represented in the original data, and it adds the inferred random effect for this group to the prediction for individuals in this group.

In the **point prediction** of the linear predictor, the unconditional expected value of u is assigned to the realizations of u for unobserved levels of non-spatial random effects (it is zero in GLMMs but not for non-gaussian random effects), and the inferred value of u is assigned in all other cases. Corresponding values of v are then deduced. This computation yields the classical "BLUP" or empirical Bayes predictor in LMMs, but otherwise it may yield less well characterized predictors, where "unconditional" v may not be its expected value when the rand family link is not identity.

There are cases where prediction without a newdata argument may give results of different length than prediction with newdata=<original data>, as for predict. Notably, for multivariate-response fits, different subsets of lines of the data may be used for each submodel depending on the availability of all variables (including the response variable) for each submodel, and the resulting fitted values from each submodel will be used from prediction; while prediction with newdata does not check the availability of a response variable.

**Intervals** computations use the relevant variance estimates plugged in a Gaussian approximation, except for the simple linear model where it uses Student's *t* distribution.

#### Value

See Details in Tpoisson for questions specific to truncated distributions.

For predict, a matrix or data frame (according to the binding argument), with optional attributes frame, intervals, predVar, fixefVar, residVar, and/or respVar, the last four holding one or more variance vector or covariance matrices. The further attribute fittedName contains the binding name, if any. The frame attribute includes information about any na.action effect on the new data.

The get\_... extractor functions call predict and extract from its result the attribute implied by the name of the extractor. By default, get\_intervals will return prediction intervals using predVar. get\_predVar with non-default which argument has the same effect as the get\_... function whose name is implied by which.

### See Also

predVar for information specific to prediction variances sensu lato, including the definitions of the four components of prediction variance, fixefVar, predVar, residVar and respVar, that can be requested through the variances argument; get\_cPredVar for a bootstrap-corrected version of get\_predVar; residVar for an alternative extractor for residual variances, more general than get\_residVar.

### **Examples**

## (2) re.form usage to remove a random effect from point prediction and variances:

```
predict(fitobject2,re.form= ~ 1 + Matern(1|longitude+latitude))
## (3) comparison of covariance matrices for two types of new data
moregroups <- grouped[1:5,]</pre>
rownames(moregroups) <- paste0("newloc",1:5)</pre>
moregroups\$grp < - rep(3,5) ## all new data belong to an unobserved third group
cov1 <- get_predVar(fitobject2,newdata=moregroups,</pre>
                     variances=list(linPred=TRUE,cov=TRUE))
moregroups$grp <- 3:7 ## all new data belong to distinct unobserved groups
cov2 <- get_predVar(fitobject2,newdata=moregroups,</pre>
                     variances=list(linPred=TRUE,cov=TRUE))
cov1-cov2 ## the expected off-diagonal covariance due to the common group in the first fit.
## Not run:
#### Other extractors:
fix_X_ZAC.object <- preprocess_fix_corr(fitobject,fixdata=blackcap)</pre>
# ... for use in multiple calls to get_predCov_var_fix():
get_predCov_var_fix(fitobject,newdata=blackcap[14,],fix_X_ZAC.object=fix_X_ZAC.object)
#### Prediction with distinct given phi's in different locations,
   as specified by a resid.model:
#
varphi <- cbind(blackcap,logphi=runif(14))</pre>
vphifit <- fitme(migStatus ~ 1 + Matern(1|longitude+latitude),</pre>
                     resid.model = list(formula=~0+offset(logphi)),
                     data=varphi, fixed=list(nu=4,rho=0.4))
# For respVar computation (i.e., response variance, often called prediction variance),
   one then also needs to provide the variables used in 'resid.model', here 'logphi':
get_respVar(vphifit,newdata=data.frame(latitude=1,longitude=1,logphi=1))
# For default 'predVar' computation (i.e., uncertainty in point prediction),
    this is not needed:
get_predVar(vphifit,newdata=data.frame(latitude=1,longitude=1))
#### point predictions and variances with new X and Z
#
if(requireNamespace("rsae", quietly = TRUE)) {
 data("landsat", package = "rsae")
 fitobject <- fitme(HACorn ~ PixelsCorn + PixelsSoybeans + (1|CountyName),</pre>
                     data=landsat[-33,])
 newXandZ <- unique(data.frame(PixelsCorn=landsat$MeanPixelsCorn,</pre>
                                 PixelsSoybeans=landsat$MeanPixelsSoybeans,
                                 CountyName=landsat$CountyName))
 predict(fitobject,newdata=newXandZ,variances = list(predVar=TRUE))
 get_predVar(fitobject, newdata=newXandZ, variances = list(predVar=TRUE))
}
```

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## End(Not run)

predVar

Prediction and response variances

## **Description**

spaMM allows computation of four variance components of prediction, returned by predict as "...Var" attributes: predVar, fixefVar, residVar, or respVar. The phrase "prediction variance" is used inconsistently in the literature. Often it is used to denote the uncertainty in the response (therefore, including the residual variance), but **spaMM** follows some literature for mixed models in departing from this usage. Here, this uncertainty is called the response variance (respVar), while prediction variance (predVar) is used to denote the uncertainty in the linear predictor (as in Booth & Hobert, 1998; see also Jeske & Harville, 1988). The respVar is the predVar plus the residual variance residVar.

Which components are returned is controlled in particular by the type and variances arguments of the relevant functions. variances is a list of booleans whose possible elements either match the possible returned components: predVar, fixefVar, residVar, or respVar; or may additionally include linPred, disp, cov, as\_tcrossfac\_list and possibly other cryptic ones.

The predict default value for all elements is NULL, which jointly translate to no component being computed, equivalently to setting all elements to FALSE. However, setting one component to TRUE may reverse the default effect for other components. In particular, by default, component predVar implies linPred=TRUE, disp=TRUE and component respVar additionally implies residVar=TRUE; in both cases, the linPred=TRUE default by default implies fixefVar=TRUE. Calling for one variance may imply that some of its components are not only computed but also returned as a distinct attribute.

By default the returned components are vectors of variances (with exceptions for some type value). To obtain covariance matrices (when applicable), set cov=TRUE. as\_tcrossfac\_list=TRUE can be used to return a list of matrices  $X_i$  such that the predVar covariance matrix equals  $\sum_i X_i X_i'$ . It thus provides a representation of the predVar that may be useful in particular when the predVar has large dimension, as the component  $X_i$ s may require less memory (being possibly non-square or sparse).

residVar=TRUE evaluates residVar the residual variance. For families without a dispersion parameter (e.g., binomial or poisson), this is as given by the variance function of the family object (in the binomial case, it is thus the variance of a single binary draw). For families with a dispersion parameter (such as  $\phi$  for gaussian or Gamma families, negative-binomial, beta), it is the residual variance as function of the dispersion parameter, whether this parameter is a single scalar or follows a more complex residual-dispersion model. Prior weights are however ignored (see the residVar etractor for the opposite feature). For the beta-binomial family, it is also the variance of a single binary draw; although this family has a residual-dispersion parameter the latter variance is not affected by it.

fixefVar=TRUE evaluates fixefVar, the variance due to uncertainty in fixed effects ( $\mathbf{X}\beta$ ).

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Computations implying linPred=TRUE will take into account the variances of the linear predictor  $\eta$ , i.e. the uncertainty in fixed effects ( $\mathbf{X}\beta$ ) and random effects ( $\mathbf{ZLv}$ ), for given dispersion parameters (see Details). For fixed-effect models, the fixefVar calculations reduces to the linPred one.

Computations implying disp=TRUE additionally include the effect of uncertainty in estimates of dispersion parameters ( $\lambda$  and  $\phi$ ), with some limitations (see Details). variances=list(predVar=TRUE), which evaluates the uncertainty of linear predictor, implies disp=TRUE by default, meaning that it includes such effects of uncertainty in dispersion parameters on the linear predictor. variances=list(respVar=TRUE) performs similarly but additionally includes the residual variance in the returned variance.

#### **Details**

fixefVar is the (co)variance of  $X\beta$ , deduced from the asymptotic covariance matrix of  $\beta$  estimates.

linPred is the prediction (co)variance of  $\eta = X\beta + Zv$  (see HLfit Details for notation, and keep in mind that new matrices may replace the ones from the fit object when newdata are used), by default computed for given dispersion parameters. It takes into account the joint uncertainty in estimation of  $\beta$  and prediction of  $\mathbf{v}$ . In particular, for new levels of the random effects, predVar computation takes into account uncertainty in prediction of  $\mathbf{v}$  for these new levels. For **prediction covariance** with a new  $\mathbf{Z}$ , it matters whether a single or multiple new levels are used: see Examples.

For computations implying disp=TRUE, prediction variance may also include a term accounting for uncertainty in  $\phi$  and  $\lambda$ , computed following Booth and Hobert (1998, eq. 19). This computation acheives its originally described purpose for a scalar residual variance ( $\phi$ ) and for several random effects with scalar variances ( $\lambda$ ). This computation ignores uncertainties in spatial correlation parameters.

The (1998) formulas for the effect of uncertainty in dispersion parameters are here also applied to the variance parameters in random-coefficient terms, but with a one-time warning. Not only this is not expected to account for the uncertainty of the correlation parameter(s) of such terms, but the result will depend on the internal representation (the "square root") of the covariance matrix, which may differ among the different fitting algorithms that may be used by **spaMM**.

respVar is the sum of predVar (pre- and post-multiplied by  $\partial \mu/\partial \eta$  for models with non-identity link) and of residVar.

These variance calculations are approximate except for LMMs, and cannot be guaranteed to give accurate results.

#### References

Booth, J.G., Hobert, J.P. (1998) Standard errors of prediction in generalized linear mixed models. J. Am. Stat. Assoc. 93: 262-272.

Jeske, Daniel R. & Harville, David A. (1988) Prediction-interval procedures and (fixed-effects) confidence-interval procedures for mixed linear models. Communications in Statistics - Theory and Methods, 17: 1053-1087, doi:10.1080/03610928808829672

```
## Not run:
# (but run in help("get_predVar"))
data("blackcap")
```

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```
fitobject <- fitme(migStatus ~ 1 + Matern(1|longitude+latitude),data=blackcap,</pre>
                        fixed=list(nu=4,rho=0.4,phi=0.05))
#### multiple controls of prediction variances
# (1) fit with an additional random effect
grouped <- cbind(blackcap,grp=c(rep(1,7),rep(2,7)))</pre>
fitobject <- fitme(migStatus ~ 1 + (1|grp) +Matern(1|longitude+latitude),</pre>
                        data=grouped, fixed=list(nu=4,rho=0.4,phi=0.05))
# (2) re.form usage to remove a random effect from point prediction and variances:
predict(fitobject,re.form= ~ 1 + Matern(1|longitude+latitude))
# (3) comparison of covariance matrices for two types of new data
moregroups <- grouped[1:5,]</pre>
rownames(moregroups) <- paste0("newloc",1:5)</pre>
moregroups\$grp <- rep(3,5) ## all new data belong to an unobserved third group
cov1 <- get_predVar(fitobject,newdata=moregroups,</pre>
                     variances=list(linPred=TRUE,cov=TRUE))
moregroups$grp <- 3:7 ## all new data belong to distinct unobserved groups
cov2 <- get_predVar(fitobject,newdata=moregroups,</pre>
                     variances=list(linPred=TRUE,cov=TRUE))
cov1-cov2 ## the expected off-diagonal covariance due to the common group in the first fit.
## End(Not run)
## see help("get_predVar") for further examples
```

pseudoR2

Pseudo R-squared

## Description

Generalization of R-squared based on likelihood ratios, called pseudo-R2 below, and variously attributed to Cragg & Uhler (1970), Cox & Snell (1989), Magee (1990) and some other authors (see comments in the References section). The null model used in the definition of R2 can be modified by the user.

# Usage

```
pseudoR2(fitobject, nullform = . ~ 1, R2fun = LR2R2, rescale=FALSE, verbose=TRUE)
```

## **Arguments**

fitobject

The fitted model object, obtained as the return value of a **spaMM** fitting func-

nullform

Mean-response formula for the null model. The default value (including only an intercept) represents the traditional choice in R2 computation for linear models. Alternative formulas (including, e.g., random effects) can be specified using either the update.formula syntax (e.g., with a '.' on the right hand side;

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note that **spaMM**'s updating conventions differ from those implemented by stats::update.formula, see update.HLfit), or a full formula (which may

be a safer syntax).

R2fun The backend function computing R2 given the fitted and null model. The default

implements the pseudo-R2. For linear models, it reduces to the canonical R2 and

the value adjusted as in summary. 1m is also returned.

rescale Boolean or formula, controlling whether and how to rescale R2 so that its max-

imum possible value is 1 (often considered for discrete-response models). If a formula, it should specify the model with maximal R2. If TRUE, rescaling is performed in a way meaningful only for binary logistic regression (see Exam-

ples for how this is implemented).

verbose Boolean; whether to display various informations about the procedure (most

notably, to warn about some potential problem in applying the default procedure

to fitobject).

### **Details**

None of the R2-like computations I am aware of helps in addressing, for the general class of models handled by **spaMM**, a well-defined inference task (comparable to, say, formally testing goodness of fit, or measuring accuracy of prediction of new data as considered for AIC). This problem has been well-known (e.g., Magee, 1990), and the canonical R2 itself for linear models is not devoid of weaknesses from this perspective (e.g., https://stats.stackexchange.com/questions/13314/is-r2-useful-or-dangerous). As a consequence, strong statements about the properties that R2 should have are difficult to follow (and this includes the claim that it should always have maximum value 1).

Given the above problems, (1) ultimately the main reason for computing R2 may be to deal with requests by misguided reviewers; (2) no attempt has been made here to implement the wide diversity of R2-like descriptors discussed in the literature. The LR2R2 backend function implements the pseudo-R2, chosen on the basis that this is the simplest general method that makes at least as much sense as any other computation I have seen; and implementation of rescaling by maximal R2 is minimal (the examples explain some of its details). LR2R2 allows adaptation of the R2 definition for mixed-effect models, by including some random effect(s) in the null model, using the nullform argument.

## Value

As returned by the function specified by argument R2fun. The default function returns a numeric vector of length 2 for linear models and a single value otherwise.

## References

Cox, D.R., Snell, E.J. (1989). The analysis of binary data (2nd ed.). Chapman and Hall. Often cited in this context, but they barely mention the topic, in an exercise p. 208-209.

Pseudo-R2 is known to go back at least to

Cragg, J. G., & Uhler, R. S. (1970). The demand for automobiles. The Canadian Journal of Economics, 3(3), 386. doi:10.2307/133656

where they already discussed its rescaling by a maximum value, in the context of binary regression.

170 random-effects

Magee, L. (1990) R2 Measures based on Wald and likelihood ratio joint significance tests. The American Statistician, 44, 250-253. doi:10.1080/00031305.1990.10475731 also often cited for the pseudo-R2, this paper reformulates some related descriptors and concisely reviews earlier literature.

Nagelkerke, N.J.D. (1991) A note on a general definition of the coefficient of determination. Biometrika, Vol. 78, No. 3. (Sep., 1991), pp. 691-692. doi:10.1093/biomet/78.3.691 details the properties of pseudo-R2 (including the way it "partitions" variation). Argues emphatically for its rescaling, for which it is often cited.

# **Examples**

```
#### Pseudo-R2 *is* R2 for linear models:
# lmfit <- lm(sr ~ pop15+pop75+dpi+ddpi , data = LifeCycleSavings)</pre>
# summary(lmfit) # Multiple R-squared = 0.3385, adjusted = 0.2797
spfit <- fitme(sr ~ pop15+pop75+dpi+ddpi , data = LifeCycleSavings)</pre>
pseudoR2(spfit) # consistent with summary(lmfit)
#### Toy example of pseudo-R2 for binary data
set.seed(123)
toydf <- data.frame(x=seq(50), y=sample(0:1,50,TRUE))</pre>
    Binary logistic regression:
binlog <- fitme(y~x, data=toydf, family=binomial())</pre>
(blR2 <- pseudoR2(binlog)) # quite low, despite the model being correct
    Rescaling by 'maximum possible' R2 for binary logistic regression:
##
pseudoR2(binlog, rescale=TRUE)
     which is acheived by silently computing the maximum possible R2 value
#
    by the following brutal but effective way:
perfbinlog <- fitme(y~I(y), data=toydf, family=binomial())</pre>
(maxblR2 <- pseudoR2(perfbinlog)) # = 0.7397...</pre>
# (this 'maximum possible' value would be modified if the null model were modified).
blR2/maxblR2
                   # again, rescaled value
##
     Same by more general syntax:
pseudoR2(binlog, rescale=y~I(y))
```

random-effects

Structure of random effects

rankinfo 171

## **Description**

The structure of random-effect models adjustable by spaMM can generally be described by the following steps.

First, independent and identically distributed (iid) random effects  ${\bf u}$  are drawn from one of the following distributions: **Gaussian** with zero mean, unit variance, and identity link; **Beta**-distributed, where  $u \sim B(1/(2\lambda), 1/(2\lambda))$  with mean=1/2, and var=  $\lambda/[4(1+\lambda)]$ ; and with logit link v=logit(u); **Gamma**-distributed random effects, where  $u \sim \text{Gamma}$  (shape=1+1/ $\lambda$ , scale=1/ $\lambda$ ): see Gamma for allowed links and further details; and **Inverse-Gamma**-distributed random effects, where  $u \sim \text{inverse-Gamma}$  for allowed links and further details.

Second, a transformation  $\mathbf{v} = f(\mathbf{u})$  is applied (this defines  $\mathbf{v}$  whose elements are still iid). By default,  $\mathbf{v} = \mathbf{u}$  for gaussian random effects but not necessarily for other distributions of random effects (see Gamma).

Third, correlated random effects are obtained as **Mv**, where the matrix **M** can describe spatial correlation between observed locations, block effects (or repeated observations in given locations), and possibly also correlations involving unobserved locations (as is often the case for autoregressive models). In most cases **M** is determined from the model formula, but it can also be controlled by **covStruct** argument. **M** takes the form **ZL** or **ZAL**, where **Z** is determined from the model formula, the optional **A** factor is given by the optional "AMatrices" attribute of argument **covStruct** of HLCor (also handled by fitme and corrHLfit), and **L** can be determined from the model formula or from **covStruct**. In particular:

- \* **Z** is typically an incidence matrix: its elements  $z_{ij}$  are 1 if the *i*th observation is affected by the *j*th element of ALb, and zero otherwise.
- \* For spatial random effects, **L** is typically the Cholesky "square root" of a correlation matrix determined by the random effect specification (e.g., Matern(...)), or given by the covStruct argument. This may be meaningful only for Gaussian random effects. Coefficients for each level of a random-coefficient model can also be represented as **Lv** where **L** is the "square root" of a correlation matrix.
- \* If there is one response value par location, **L** for a spatial random effect is thus a square matrix whose dimension is the number of observations. Alternatively, several observations may be taken in the same location, and a matrix **Z** (automatically constructed) tells which element of **Lv** affects each observation. The linear predictor then contains a term of the form **ZLv**, where dim(Z) is (number of observations, number of locations).
- \* in IMRF random effects (IMRF for Interpolated Markov Random Fields), the realized random effects in response locations are defined as linear combinations **ALv** of random effects **Lv** in distinct locations. In that case the dimension of **L** is the number of such distinct locations, an automatically constructed **A** matrix maps them to the observed locations, and **Z** again maps them to possibly repeated observations in observed locations.

172 rankinfo

## **Description**

By default, fitting functions in spaMM check the rank of the design matrix for fixed effects, as stats::lm or stats::glm do (but not, say, nlme::lme). This computation can be quite long. To save time when fitting different models with the same fixed-effect terms to the same data, the result of the check can be extracted from a return object by get\_rankinfo(), and can be provided as argument control.HLfit\$rankinfo to another fit. Alternatively, the check will not be performed if control.HLfit\$rankinfo is set to NA.

## Usage

```
get_rankinfo(object)
```

## **Arguments**

object

An object of class HLfit, as returned by the fitting functions in spaMM.

#### **Details**

The check is performed by a call to qr() methods for either dense or sparse matrices. If the design matrix is singular, a set of columns from the design matrix that define a non-singular matrix is identified. Note that different sets may be identified by sparse- and dense-matrix qr methods.

### Value

A list with elements rank, whichcols (a set of columns that define a non-singular matrix), and method (identifying the algorithm used).

register\_cF 173

register\_cF

Declare corrFamily constructor for use in formula

## **Description**

register\_cF registers the name of a new corrFamily constructor so that it can be used as the keyword of a random effect in a formula (as in  $y \sim 1 + ARp()$ ). unregister\_cF cancels this.

## Usage

```
register_cF(corrFamilies = NULL, reset = FALSE)
unregister_cF(corrFamilies)
```

# Arguments

corrFamilies N

NULL, or character vector of names of corrFamily constructors.

reset

Boolean. Set it to TRUE in order to reset the list of registered constructors to the **spaMM** built-in default, before registering the ones specified by corrFamilies.

#### Value

No value; operates through side-effects on internal variables.

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resid.model

Structured dispersion models

## **Description**

The resid.model argument of fitting functions can be used to specify a model for a residual-dispersion parameter of various response families, that is, either

- (1) the  $\phi$  parameter of the gaussian and Gamma GLM families;
- (2a) the dispersion parameter of some other GLM families, such as the shape parameter of the negbin1 and negbin2 families; or
- (2b) the dispersion parameter of some other (non-GLM) response families, such as the precision parameter of the beta response family.

This documentation is more specifically for case (2). Case (1) is more specifically documented as phi-resid.model.

In case (2) the model for the dispersion parameter is constrained as a fixed-effect model, of the form dispersion parameter =  $\exp(\mathbf{X}\beta + \text{offset})$ ,

and specified using the standard formula syntax. Random effects cannot be included, in contrast to dispersion models for case (1).

#### Usage

```
# 'resid.model' argument of fitme() and fitmv()
```

### **Arguments**

The resid.model for case (2) is simply a formula (without left-hand side) for the logarithm of the dispersion parameter. Fixed  $\beta$  values can be specified through the rdisPars element of the fixed argument in the fitme call (or through the fixed argument of each submodel of a fitmv call). Likewise, initial values can be specified through the init argument.

#### **Details**

In case (2) a fixed "heteroscedastic" model can also be specified directly through the family specification, e.g., family=negbin1(shape=<vector>) where the vector has the length of the response vector, but this may not be suitable if the model is to be used for prediction purposes (where the residual-dispersion model should be specified in such a way that one can "predict" new dispersion values from it).

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The design matrix for the specified model is internally rescaled to avoid numerical problems. That means that there is no need to rescale the predictor variable, even if it tends to take large (cf 'population' variable in the Examples) of small values (this is also true for fixed-effect predictors of the mean-response model).

#### Value

The fit results for the residual model are accessible through the summary and various extractors. In particular, the get\_fittedPars extractor will by default include in its return value the rdisPars element, which is here the vector of fitted  $\beta$  coefficients. residVar(., which="fam\_parm") will return the vector of fitted values of the dispersion parameter.

## **Examples**

```
data("scotlip")
if (spaMM.getOption("example_maxtime")>3) {
  (toyfit <- fitme(cases~1+(1|id),family=negbin1(), data=scotlip, resid.model = ~ population))
# => This toy example is a bit challenging to fit because the data set is small and
# individual-level variation is here described both by a random effect
# and by a two-parameter negbin1 residual variation. The fit might often stop
# at a local maximum of the logLik in such cases (although there is no evidence
# that this is presently the case).
}
```

residuals.HLfit

Extract model residuals

### **Description**

Extracts several types of residuals from an object of class HLfit. Note that the default type ("deviance") of returned residuals differs from the default (response residuals) of equivalent functions in base R.

# Usage

```
## S3 method for class 'HLfit'
residuals(object,
  type = c("deviance", "pearson", "response", "working", "std_dev_res"), force=FALSE, ...)
```

## **Arguments**

object	An object of class HLfit, as returned by the fitting functions in spaMM.
type	The type of residuals which should be returned. See Details for additional information.
force	Boolean: to force recomputation of the "std_dev_res" residuals even if they are available in the object, for checking purposes.
	For consistency with the generic.

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#### **Details**

The four types "deviance" (default), "pearson", "response" are "working" are, for GLM families, the same that are returned by residuals.glm. "working" residuals may be returned only for fixed-effect models. "deviance" residuals are the signed square root of those returned by dev\_resids when there are no prior weights.

In the presence of prior weights, what the standard extractors do is often a matter of confusion and **spaMM** has not always been consistent with them. For a gaussian-response GLM (see Examples) stats::deviance.lm calls weighted.residuals() which returns *unscaled* deviance residuals weighted by prior weights. Unscaled deviance residuals are defined in McCullagh and Nelder 1989, p. 34 and depend on the response values and fitted values but not on the canonical  $\phi$  parameter, and prior weights are not considered. weighted.residuals() still ignores  $\phi$  but accounts for prior weights. This means that different residuals(q0 and deviance(q0 will be returned for equivalent fits with different parametrizations of the residual variance (as produced by q0, family=gaussian, weights=rep(2,nrow(data>)) versus the q0 without weights). residuals(q0 without weights). residuals(q1 below this behavior. By contrast, dev\_resids(q1 below the unscaled deviance residuals by default.

Following Lee et al. (2006, p.52), the standardized deviance residuals returned for type="std\_dev\_res" are defined as the deviance residuals divided by  $\phi\sqrt(1-q)$ , where the deviance residuals are defined as for a GLM,  $\phi$  is the dispersion parameter of the response family (a vector of values, for heteroscedastic cases), and q is a vector of leverages given by hatvalues(., type="std") (see hatvalues for details about these specific standardizing leverages).

Some definitions must be extended for non-GLM response families. In the latter case, the deviance residuals are as defined in Details of llm.fit (there is no concept of unscaled residuals here, nor indeed of scaled ones since the residual dispersion parameter is not generally a scale factor, but the returned deviance residuals for non-GLMs are analogous to the scaled ones for GLMs as they depend on residual dispersion). "std\_dev\_res" residuals are defined from them as shown above for GLM response families, with the additional convention that  $\phi=1$  (since the family's own residual dispersion parameter already enters in the definition of deviance residuals for non-GLM families). Pearson residuals and response residuals are defined as in stats::residuals.glm. The "working" residuals are defined for each response as  $-[d\log(clik)/d\eta]/[d^2\log(clik)/d\eta^2]$  where clik is the conditional likelihood.

### Value

A vector of residuals

### References

Lee, Y., Nelder, J. A. and Pawitan, Y. (2006). Generalized linear models with random effects: unified analysis via h-likelihood. Chapman & Hall: London.

```
data("wafers")
fit <- fitme(y ~X1+(1|batch) ,data=wafers, init=list(phi=NaN)) # : this 'init'
# implies that standardized deviance residuals are saved in the
# fit result, allowing the following comparison:</pre>
```

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```
r1 <- residuals(fit, type="std_dev_res") # gets stored value
r2 <- residuals(fit, type="std_dev_res", force=TRUE) # forced recomputation
if (diff(range(r1-r2))>1e-14) stop()
#####
## Not run:
glmfit \leftarrow glm(I(y/1000)^X1, family=gaussian(), data=wafers)
                              3...
deviance(glmfit) #
                                                           (a)
                              3...
sum(residuals(glmfit)^2) #
                                                           (b)
# Same model, with different parametrization of residual variance
glmfit2 <- glm(I(y/1000)~X1, family=gaussian(), data=wafers, weights=rep(2,198))</pre>
deviance(glmfit2) #
                              6...
                                                           (c)
                                                           (d)
sum(residuals(glmfit2)^2) # 6...
# Same comparison but for HLfit objects:
spfit <- fitme(I(y/1000)~X1, family=gaussian(), data=wafers)</pre>
deviance(spfit) #
                              3...
sum(residuals(spfit)^2) #
                              3...
                                                           (f)
sum(dev_resids(spfit)) #
                              3...
spfit2 \leftarrow fitme(I(y/1000)^XI, family=gaussian(), data=wafers, prior.weights=rep(2,198))
                                                           (g) \sim (c,d) # post v4.2.0
deviance(spfit2) #
                              6...
                                                           (h) \sim (c,d)
sum(residuals(spfit2)^2) #
                              6...
sum(dev_resids(spfit2)) #
                              3...
# Unscaled residuals should no depend on arbitrarily fixed residual variance:
spfit3 \leftarrow fitme(I(y/1000)^XI, family=gaussian(), data=wafers, fixed=list(phi=2),
                prior.weights=rep(2,198))
                                                           (i) ~ (g)
deviance(spfit3) #
                              6...
                                                           (k) \sim (h)
sum(residuals(spfit3)^2) #
                              6...
sum(dev_resids(spfit3)) #
## End(Not run)
```

residVar

Residual variance extractor

## **Description**

Extracts from a fit object the residual variance or, depending on the which argument, a family dispersion parameter phi (which is generally not the residual variance itself except for gaussian-response models without prior weights), or a vector of values of the dispersion parameter, or further information about the residual variance model.

For gaussian and Gamma response families, the return values for which = "var" and "phi" include prior weights, if any.

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### Usage

```
residVar(object, which = "var", submodel = NULL, newdata = NULL)
```

#### **Arguments**

object An object of class HLfit, as returned by the fitting functions in spaMM.

which Character: "var" for the fitted residual variances, "phi" for the fitted phi values,

"fam\_parm" for the dispersion parameter of COMPoisson, negbin1, negbin2, beta\_resp or betabin families, "fit" for the fitted residual model (a GLM or a mixed model for residual variances, if not a simpler object), and "family" or

"formula" for such properties of the residual model.

submodel integer: the index of a submodel, if object is a multivariate-response model

fitted by fitmv. This argument is mandatory for all which values except "var"

and "phi".

newdata **Either** NULL, a matrix or data frame, or a numeric vector. See predict.HLfit

for details.

#### Value

which="var" (default) and "phi" always return a vector of residual variances (or, alternatively, phi values) of length determined by the newdata and submodel arguments.

which="fit" returns an object of class HLfit, glm, or a single scalar depending on the residual dispersion model (which="fit" is the option to be used to extract the scalar phi value).

which="fam\_parm" returns either NULL (for families without such a parameter), a vector (if a resid.model was specified for relevant families), a single scalar (relevant families, without resid.model), or a list of such objects (for multivariate-response models).

Other which values return an object of class family or formula as expected.

## See Also

get\_residVar is a alternative extractor of residual variances with different features inherited from get\_predVar. In particular, it is more suited for computing the residual variances of new realizations of a fitted model, not accounting for prior weights used in fitting the model (basic examples of using the **IsoriX** package provide a context where this is the appropriate design decision). By contrast, residVar aims to account for prior weights.

```
# data preparation: simulated trivial life-history data
set.seed(123)
nind <- 20L
u <- rnorm(nind)
lfh <- data.frame(
  id=seq_len(nind), id2=seq_len(nind),
  feco= rpois(nind, lambda = exp(1+u)),
  growth=rgamma(nind,shape=1/0.2, scale=0.2*exp(1+u)) # mean=exp(1+u), var= 0.2*mean^2
)
# multivariate-response fit
fitlfh <- fitmv(submodels=list(list(feco ~ 1+(1|id), family=poisson()),</pre>
```

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salamander

Salamander mating data

## **Description**

Data from a salamander mating experiment discussed by McCullagh and Nelder (1989, Ch. 14). Twenty males and twenty females from two populations (Rough Butt and Whiteside) were each paired with 6 individuals from their own or from the other population. The experiments were later published by Arnold et al. (1996).

## Usage

```
data("salamander")
```

#### **Format**

The data frame includes 360 observations on the following variables:

Female Index of the female;

Male Index of the male;

Mate Whether the pair successfully mated or not;

**TypeF** Population of origin of female;

**TypeM** Population of origin of male;

Cross Interaction term between TypeF and TypeM;

Season A factor with levels Summer and Fall;

**Experiment** Index of experiment

#### Source

The data frame was borrowed from the HGLMMM package (Molas and Lesaffre, 2011), version 0.1.2.

## References

Arnold, S.J., Verrell, P.A., and Tilley S.G. (1996) The evolution of asymmetry in sexual isolation: a model and a test case. Evolution 50, 1024-1033.

McCullagh, P. and Nelder, J.A. (1989). Generalized Linear Models, 2nd edition. London: Chapman & Hall.

Molas, M., Lesaffre, E. (2011) Hierarchical Generalized Linear Models: The R Package HGLMMM. Journal of Statistical Software 39, 1-20.

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### **Examples**

scotlip

Lip cancer in Scotland 1975 - 1980

## Description

This data set provides counts of lip cancer diagnoses made in Scottish districts from 1975 to 1980, and additional information relative to these data from Clayton and Kaldor (1987) and Breslow and Clayton (1993). The data set contains (for each district) counts of disease events and estimates of the fraction of the population involved in outdoor industry (agriculture, fishing, and forestry) which exposes it to sunlight.

data("scotlip") actually loads a data frame, scotlip, and an adjacency matrix, Nmatrix, between 56 Scottish districts, as given by Clayton and Kaldor (1987, Table 1).

## Usage

```
data("scotlip")
```

## **Format**

The data frame includes 56 observations on the following 7 variables:

gridcode alternative district identifier.

id numeric district identifier (1 to 56).

district district name.

cases number of lip cancer cases diagnosed 1975 - 1980.

population total person years at risk 1975 - 1980.

**prop.ag** percent of the population engaged in outdoor industry.

expec offsets considered by Breslow and Clayton (1993, Table 6, 'Exp' variable)

The rows are ordered according to gridcode, so that they match the rows of Nmatrix.

### References

Clayton D, Kaldor J (1987). Empirical Bayes estimates of age-standardized relative risks for use in disease mapping. Biometrics, 43: 671 - 681.

Breslow, NE, Clayton, DG. (1993). Approximate Inference in Generalized Linear Mixed Models. Journal of the American Statistical Association: 88 9-25.

seaMask 181

# **Examples**

```
data("scotlip")
fitme(cases~I(log(expec)), data=scotlip, adjMatrix=Nmatrix, family=poisson)
## see 'help(autoregressive)' for additional examples involving 'scotlip'.
```

seaMask

Masks of seas or lands

# **Description**

These convenient masks can be added to maps of (parts of) the world to mask map information for these areas.

However, many other tools may be available since this documentation was conceived. See e.g. the **rnaturalearth** package, used to provide a sea mask in an example for filled.mapMM

# Usage

```
data("seaMask")
data("landMask")
# data("worldcountries") # deprecated and removed
# data("oceanmask") # deprecated and removed
```

#### **Format**

seaMask and landMask are data frames with two variables, x and y for longitude and latitude. Its contents are suitable for use with polypath: they define different polygones, each separated by a row of NAs.

worldcountries and oceanmask were sp::SpatialPolygonsDataFrame objects previously included in spaMM (see Details for replacement). Such objects were useful for creating land masks for different geographical projections.

## **Details**

The removed objects worldcountries and oceanmask were suitable for plots involving geographical projections not available through map, and more generally for raster plots. A land mask could be produced out of worldcountries by filling the countries, as by fill="black" in the code for country.layer in the Examples in https://gitlab.mbb.univ-montp2.fr/francois/spamm-ref/-/blob/master/vignettePlus/example\_raster.html. These objects may now be available through the same web page, but a better place to look for the same functionality is the IsoriX package (objects CountryBorders and OceanMask).

seaMask and landMask were created from the world map in the maps package. polypath requires polygons, while map(interior=FALSE,plot=FALSE) returns small segments. landMask is the result of reconnecting the segments into full coastlines of all land blocks.

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#### See Also

https://gitlab.mbb.univ-montp2.fr/francois/spamm-ref/-/blob/master/vignettePlus/example\_raster.html for access to, and use of worldcountries and oceanmask; https://cran.r-project.org/package=IsoriX for replacement CountryBorders and OceanMask for these objects.

# **Examples**

```
## Predicting behaviour for a land bird: simplified fit for illustration
data("blackcap")
bfit <- fitme(migStatus ~ means+ Matern(1|longitude+latitude),data=blackcap,</pre>
               fixed=list(lambda=0.5537,phi=1.376e-05,rho=0.0544740,nu=0.6286311))
## the plot itself, with a sea mask,
## and an ad hoc 'pointmask' to see better the predictions on small islands
#
def_pointmask <- function(xy,r=1,npts=12) {</pre>
 theta <- 2*pi/npts *seq(npts)</pre>
 hexas <- lapply(seq(nrow(xy)), function(li){</pre>
    p <- as.numeric(xy[li,])</pre>
   hexa <- cbind(x=p[1]+r*cos(theta),y=p[2]+r*sin(theta))</pre>
    rbind(rep(NA,2),hexa) ## initial NA before each polygon
 })
 do.call(rbind, hexas)
11 <- blackcap[,c("longitude","latitude")]</pre>
pointmask \leftarrow def_pointmask(ll[c(2,4,5,6,7),],r=0.8) ## small islands only
if (spaMM.getOption("example_maxtime")>1) {
 data("seaMask")
 filled.mapMM(bfit,add.map=TRUE,
             plot.title=title(main="Inferred migration propensity of blackcaps",
                                xlab="longitude",ylab="latitude"),
             decorations=quote(points(pred[,coordinates],cex=1,pch="+")),
             plot.axes=quote({axis(1);axis(2);
                         polypath(rbind(seaMask,pointmask),border=FALSE,
                                  col="grey", rule="evenodd")
             }))
}
```

seeds

Seed germination data

## **Description**

A classic toy data set, "from research conducted by microbiologist Dr P. Whitney of Surrey University. A batch of tiny seeds is brushed onto a plate covered with a certain extract at a given dilution. The numbers of germinated and ungerminated seeds are subsequently counted" (Crowder, 1978). Two seed types and two extracts are here considered in a 2x2 factorial design.

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## Usage

```
data("seeds")
```

#### **Format**

The data frame includes 21 observations on the following variables:

```
plate Factor for replication;
```

**seed** Seed type, a factor with two levels O73 and O75;

extract Root extract, a factor with two levels Bean and Cucumber;

- r Number of seeds that germinated;
- n Total number of seeds tested

#### **Source**

```
Crowder (1978), Table 3.
```

#### References

Crowder, M.J., 1978. Beta-binomial anova for proportions. Appl. Statist., 27, 34-37.

Y. Lee and J. A. Nelder. 1996. Hierarchical generalized linear models (with discussion). J. R. Statist. Soc. B, 58: 619-678.

# **Examples**

 ${\tt setNbThreads}$ 

Parallel computations in fits

## **Description**

A few steps of fitting can be parallelized. Currently it is possible to control the use of multiple threads by OpenMP by the Eigen library. By default only one thread will be used, but this may be modified by using control. HLfit\$NbThreads in a fitting function's arguments, as in

```
avail_thr <- parallel::detectCores(logical=FALSE) - 1L
fitme(., control.HLfit=list(NbThreads=max(avail_thr, 1L)))
```

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This control is distinct from that of post-fit steps such as bootstraps where some parallel computations are controlled e.g. the nb\_cores argument of spaMM\_boot. In cases where post-fits computation imply refits of models (as is typical of parametric bootstraps), the two parallelizations should not be combined, and the **spaMM** code for post-fit operations will in principle automatically take care of this.

According to https://cran.r-project.org/doc/manuals/r-devel/R-exts.html#OpenMP-support, using openMP may decrease the precision of some computations, and may be less efficient under Windows; and according to https://eigen.tuxfamily.org/dox/TopicMultiThreading.html only a few Eigen computations will benefit from such parallelisation, mainly the dense matrix products. **spaMM** will *suggest* using parallelisation when random effects have many levels and dense-correlation methods are selected (see algebra), that is mainly for geostatiscal models with many locations. Speed gains appear moderate, as the slowest steps are not parallelized.

simulate.HLfit

Simulate realizations of a fitted model.

## **Description**

From an HLfit object, simulate.HLfit function generates new samples given the estimated fixed effects and dispersion parameters. Simulation may be unconditional (the default, useful in many applications of parametric bootstrap), or conditional on the predicted values of random effects, or may draw from the conditional distribution of random effects given the observed response. Simulations may be run for the original sampling design (i.e., original values of fixed-effect predictor variables and of random-effect levels, including spatial locations if relevant), or for a new design as specified by the newdata argument.

simulate4boot is a wrapper around simulate. HLfit that can be used to precompute the bootstrap samples to be used by spaMM\_boot or spaMM2boot through their boot\_samples argument (and is called internally by these functions when boot\_samples is NULL).

simulate\_ranef will only simulate and return a vector of random effects, more specifically some elements of the **b** vector appearing in the standard form offset+  $\mathbf{X}\beta$  +  $\mathbf{Z}$  **b** for the linear predictor.

# Usage

simulate.HLfit 185

## **Arguments**

object The return object of HLfit or similar function.

nsim number of response vectors to simulate. Defaults to '1'.

seed A seed for set. seed. If such a value is provided, the initial state of the random

number generator at a global level is restored on exit from simulate.

newdata A data frame closely matching the original data, except that response values are

not needed. May provide new values of fixed predictor variables, new spatial locations, new individuals within a block, or new values of the LHS in random-

effect terms of the form (<LHS>|<RHS>).

prior.weights Prior weights that may be substituted to those of the original fit, with the same

effect on the residual variance. See Details for the definition of the default when newdata are provided. For multivariate-response fits, this is a list with one element per submodel, each element being a vector whose size is the number of response levels to be simulated for each submodel (the object\$prior.weights

provides an example).

sizes A vector of sample sizes to simulate in the case of a binomial or betabin fit.

See Details for the definition of the default when newdata are provided. For multivariate-response fits, the sizes argument should contain elements for response levels for all submodels whatever their response families (e.g. for submodels with families and response levels poisson: 3 and binomial: 2, respectively, the sizes vector should contain 5 elements, e.g. 1 1 1 5 10, only the last

two of which having nontrivial meaning).

re. form formula for random effects to condition on. Default behaviour depends on the

type argument. The joint default is the latter's default, i.e., unconditional simulation. re.form is currently ignored when type="predVar" (with a warning). Otherwise, re.form=NULL conditions on all random effects (as type="residual" does), and re.form=NA conditions on none of the random effects (as type="marginal").

or re.form=~0 do).

type character string specifying which uncertainties are taken into account in the lin-

ear predictor and notably in the random effect terms. Whatever the type, the residual variance is always accounted in the simulation output. "marginal" accounts for the marginal variance of the random effect (and, by default, also for the uncertainty in fixed effects); "predVar" accounts for the conditional distribution of the random effects given the data (see Details); and "residual" should perhaps be "none" as no uncertainty is accounted in the linear predictor:

the simulation variance is only the residual variance of the fitted model.

conditional Obsolete and will be deprecated. Boolean; TRUE and FALSE are equivalent to

type="residual" and type="marginal", respectively.

verbose Either a single boolean (which determines verbose[["type"]], or a vector of

booleans with possible elements "type" (to display basic information about the

type of simulation) and "showpbar" (see predict(., verbose)).

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resp\_testfn NULL, or a function that tests a condition which simulated samples should sat-

isfy. This function takes a response vector as argument and return a boolean

(TRUE indicating that the sample satisfies the condition).

phi\_type Character string, either "predict" or one of the values possible for type. This

controls the residual variance parameter  $\phi$ . The default is to use predicted  $\phi$  values from the fit, which are the fitted  $\phi$  values except when a structured-dispersion model is involved together with non-NULL newdata. However, when a structured-dispersion model is involved, it is also possible to simulate new  $\phi$  values, and for a mixed-effects structured-dispersion model, the same types of simulation controlled by type for the mean response can be performed as controlled by phi\_type. For a fixed-effects structured-dispersion model, these types cannot be distinguished, and any phi\_type distinct from "predict" will imply simu-

lation under the fixed-effect model (see Examples).

variances Used when type="predVar": see Details.

... For simulate4boot, further arguments passed to simulate.HLfit (e.g., newdata).

For simulate. HLfit, further arguments only passed to predict in a specula-

tive bit of code (see Details).

which Integer, or integer vector: the random effect(s) (indexed as ordered as in the

model formula) to be simulated. If NULL, all of them are simulated.

showpbar Controls display of progress bar. See barstyle option for details.

#### **Details**

type="predVar" accounts for the uncertainty of the linear predictor, by drawing new values of the predictor in a multivariate gaussian distribution with mean and covariance matrix of prediction. In this case, the user has to provide a variances argument, passed to predict, which controls what goes into this covariance matrix. For example, with variances=list(linPred=TRUE, disp=TRUE)), the covariance matrix takes into account the joint uncertainty in the fixed-effect coefficients and of any random effects given the response and the point estimates of dispersion and correlation parameters ("linPred" variance component), and in addition accounts for uncertainty in the dispersion parameters (effect of "disp" variance component as further described in predict.HLfit). The total simulation variance is then the response variance. Uncertainty in correlation parameters (such a parameters of the Matern family) is not taken into account. The "linPred" uncertainty is known exactly in LMMs, and otherwise approximated as a Gaussian distribution with mean vector and covariance matrix given as per the Laplace approximation.

type="(ranef|response)" can be viewed as a special version of type="predVar" where variances=list(linPred=TRUE, disp=FALSE)) and only the uncertainty in the random effects is taken into account.

A full discussion of the merits of the different types is beyond the scope of this documentation, but these different types may not all be useful. type="marginal" is typically used for computation of confidence intervals by parametric bootstrap methods. type="residual" is used by get\_cPredVar for its evaluation of a bias term. The other types may be used to simulate the uncertainty in the random effects, conditionally on the data, and may therefore be more akin to the computation of prediction intervals conditionally on an (unknown but inferred) realization of the random effects. But these should presumably not be used in a bootstrap computation of such intervals, as this would represent a double accounting of the uncertainty that the bootstrap aims to quantify.

There are cases where simulation without a newdata argument may give results of different length than simulation with newdata=<original data>, as for predict.

When newdata are provided but new values of prior.weights or sizes are missing, new values of these missing arguments are guessed, and warnings may be issued depending on the kind of guess made for response families dependent on such arguments. The prior.weights values used in the fit are re-used without warning when such values were identical (generally, unit) for all response values, and labelled as such in the object\$prior.weights. Unit weights will be used otherwise, with a warning. Unit binomial sizes will be used, with a warning, whenever there are newdata.

#### Value

simulate. HLfit returns a vector (if nsim=1) or a matrix with nsim columns, each containing simulated responses (or simulated random effects, for simulated\_ranef()). For multivariate-response simulations, an nobs attribute gives the number of responses for each submodel if no resp\_testfn was applied.

simulate4boot returns a list with elements

**bootreps** the result of simulate. HLfit as a matrix with nsim columns;

**RNGstate** the state of .Random. seed at the beginning of the sample simulation.

The simulate. HLfitlist method returns a list of simulated responses.

# **Examples**

spaMM

Inference in mixed models, in particular spatial GLMMs

# Description

Fits a range of mixed-effect models, including those with spatially correlated random effects. The random effects are either Gaussian (which defines GLMMs), or other distributions (which defines the wider class of hierarchical GLMs), or simply absent (which makes a LM or GLM). Multivariate-response models can be fitted by the fitmv function. Other models can be fitted by fitme. Also available are previously conceived fitting functions HLfit (sometimes faster, for non-spatial models), HLCor (sometimes faster, for conditional-autoregressive models and fixed-correlation models),

and corrHLfit (now of lesser interest). A variety of post-fit procedures are available for prediction, simulation and testing (see, e.g., fixedLRT, simulate and predict).

A variety of special syntaxes for fixed effects, such as poly, splines::ns or bs, or lmDiallel::GCA, may be handled natively although some might not be fully handled by post-fit procedures such as predict. poly is fully handled. lmDiallel::GCA cannot be due to its inherent limitations, but see X.GCA for a more functional alternative for diallel/multi-membership fixed-effect terms. Note that packages implementing these terms must be attached to the search list as :: will not be properly understood in a formula.

Both maximum likelihood (ML) and restricted likelihood (REML) can be used for linear mixed models, and extensions of these methods using Laplace approximations are used for non-Gaussian random response. Several variants of these methods discussed in the literature are included (see Details in HLfit), the most notable of which may be "PQL/L" for binary-response GLMMs (see Example for arabidopsis data). PQL methods implemented in spaMM are closer to (RE)ML methods than those implemented in MASS::glmmPQL.

#### **Details**

The standard response families gaussian, binomial, poisson, and Gamma are handled, as well as negative binomial (see negbin1 and negbin2), beta (beta\_resp), beta-binomial (betabin), zero-truncated poisson and negative binomial and Conway-Maxwell-Poisson response (see Tpoisson, Tnegbin and COMPoisson). A multi family look-alike is also available for multinomial response, with some constraints.

The variance parameter of residual error is denoted  $\phi$  (phi): this is the residual variance for gaussian response, but for Gamma-distributed response, the residual variance is  $\phi\mu^2$  where  $\mu$  is expected response. A (possibly mixed-effects) linear predictor for  $\phi$ , modeling heteroscedasticity, can be considered (see Examples).

The package fits models including several nested or crossed random effects, including autocorrelated ones. An interface is being developed allowing users to implement their own parametric correlation models (see corrFamily), beyond the following ones which are built in **spaMM**:

- \* geostatistical (Matern, Cauchy),
- \* interpolated Markov Random Fields (IMRF, MaternIMRFa),
- \* autoregressive time-series (AR1, ARp, ARMA),
- \* conditional autoregressive as specified by an adjacency matrix,
- \* pairwise interactions with individual-level random effects, such as diallel experiments (diallel),
- \* or any fixed correlation matrix (corrMatrix).

GLMMs and HGLMs are fit via Laplace approximations for (1) the marginal likelihood with respect to random effects and (2) the restricted likelihood (as in REML), i.e. the likelihood of random effect parameters given the fixed effect estimates. All handled models can be formulated in terms of a linear predictor of the traditional form offset+  $\mathbf{X}\beta$  +  $\mathbf{Z}$  b, where  $\mathbf{X}$  is the design matrix of fixed effects,  $\beta$  (beta) is a vector of fixed-effect coefficients,  $\mathbf{Z}$  is a "design matrix" for the random effects (which is instead denoted  $\mathbf{M}$ = $\mathbf{Z}\mathbf{A}\mathbf{L}$  elsewhere in the package documentation), and  $\mathbf{b}$  a vector of random effect values. The general structure of  $\mathbf{M}\mathbf{b}$  is described in random-effects.

Gaussian and non-gaussian random effects can be fitted. Different **gaussian** random-effect terms are handled, with the following effects:

\* (1|<RHS>), for non-autocorrelated random effects as in lme4;

\* (<LHS>|<RHS>), for random-coefficient terms as in lme4, \*and additional terms depending on the <LHS> type\* (further detailed below);

- \* (<LHS> || <RHS>) is interpreted as in lme4: any such term is immediately converted to ( (1|<RHS>) + (0+<LHS>|<RHS>) ). It should be counted as two random effects for all purposes (e.g., for fixing the variances of the random effects). However, this syntax is useless when the LHS includes a factor (see help('lme4::expandDoubleVerts')).
- \* <prefix>(1|<RHS>), to specify autocorrelated random effects, e.g. Matern(1|long+lat).
- \* \* \* can be used to alter the
  autocorrelated random effect as detailed below.

Different LHS types of **gaussian** (<LHS>|<RHS>) random-effect terms are handled, with the following effects:

- \* <logical> (TRUE/FALSE): affects only responses for which <LHS> is TRUE.
- \* <factor built from a logical>: same a <logical> case;
- \* <factor not built from a logical>: random-coefficient term as in lme4;
- \* 0 + <factor not built from a logical>: same but contrasts are not used;
- \* factors specified by the mv(...) expression, generate random-coefficient terms specific to multivariate-response models fitted by fitmv() (see help("mv")). 0 + mv(...) has the expected effect of not using contrasts;
- \* <numeric> (but not '0+<numeric>'): random-coefficient term as in lme4,
   with 2\*2 covariance matrix of effects on Intercept and slope;
- \* 0 + <numeric>: no Intercept so no covariance matrix (random-slope-only term);

The '0 + <numeric>' effect is achieved by direct control of the elements of the incidence matrix  $\mathbf{Z}$  through the <LHS> term: for numeric z, such elements are multiplied by z values, and thus provide a variance of order O(z squared).

If one wishes to fit uncorrelated group-specific random-effects with distinct variances for different groups or for different response variables, three syntaxes are thus possible. The most general, suitable for fitting several variances (see GxE for an example), is to fit a  $(0 + \langle \text{factor} \rangle | \langle \text{RHS} \rangle)$  random-coefficient term with correlation(s) fixed to 0. Alternatively, one can define **numeric** (011) variables for each group (as as.numeric( $\langle \text{boolean for given group membership} \rangle)$ ), and use each of them in a 0 +  $\langle \text{numeric} \rangle$  LHS (so that the variance of each such random effect is zero for response not belonging to the given group). See lev2bool for various ways of specifying such indicator variables for several levels.

\* The terms are \*not\* composite random effects when the non-'1' LHS type is boolean or factor-from-boolean, a just illustrated, but also 0+<numeric>: for example, Matern(0+<numeric>|.)

represents an autocorrelated random-slope (only) term or, equivalently, a direct specification of heteroscedasticity of the Matérn random effect.

\* By contrast, Matern(<numeric>|.) implies estimating a random-coefficient covariance matrix and thus defines a composite random effects, as does an LHS that is a factor constructed from numeric or character levels.

Composite random effects can be fitted in principle for all "prefixes", including for <corrFamily> terms. In practice, this functionality has been checked for Matern, corrMatrix, AR1 and the ARp-corrFamily term. In these terms, the <.> %in% <.> form of nested random effect is allowed.

The syntax (z-1|.), for **numeric** z only, can also be used to fit **some heteroscedastic non-Gaussian** random effects. For example, a Gamma random-effect term (wei-1|block) specifies an heteroscedastic Gamma random effect u with constant mean 1 and variance wei^2  $\lambda$ , where  $\lambda$  is still the estimated variance parameter. See Details of negbin for a possible application. Here, this effect is not implemented through direct control of  $\mathbf{Z}$  (multiplying the elements of an incidence matrix  $\mathbf{Z}$  by wei), as this would have a different effect on the distribution of the random effect term. (z|.) is not defined for *non-Gaussian* random effects. It could mean that a correlation structure between random intercepts and random slopes for (say) Gamma-distributed random effects is considered, but such correlation structures are not well-specified by their correlation matrix.

## Author(s)

spaMM was initially published by François Rousset and Jean-Baptiste Ferdy, and is continually developed by F. Rousset and tested by Alexandre Courtiol.

#### References

Lee, Y., Nelder, J. A. and Pawitan, Y. (2006). Generalized linear models with random effects: unified analysis via h-likelihood. Chapman & Hall: London.

Rousset F., Ferdy, J.-B. (2014) Testing environmental and genetic effects in the presence of spatial autocorrelation. Ecography, 37: 781-790. doi:10.1111/ecog.00566

#### See Also

See the test directory of the package for many additional examples of **spaMM** usage beyond those from the formal documentation.

See fitme for multivariate-response models.

# **Examples**

```
data("wafers")
data("scotlip") ## loads 'scotlip' data frame, but also 'Nmatrix'

## Linear model
fitme(y ~ X1, data=wafers)

## GLM
fitme(y ~ X1, family=Gamma(log), data=wafers)
fitme(cases ~ I(log(population)), data=scotlip, family=poisson)

## Non-spatial GLMMs
```

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```
fitme(y ~ 1+(1|batch), family=Gamma(log), data=wafers)
fitme(cases ~ 1+(1|gridcode), data=scotlip, family=poisson)
# Random-slope model (mind the output!)
fitme(y\sim X1+(X2|batch), data=wafers, method="REML")
## Spatial, conditional-autoregressive GLMM
if (spaMM.getOption("example_maxtime")>2) {
 fitme(cases ~ I(log(population))+adjacency(1|gridcode), data=scotlip, family=poisson,
        adjMatrix=Nmatrix) # with adjacency matrix provided by data("scotlip")
# see ?adjacency for more details on these models
## Spatial, geostatistical GLMM:
# see e.g. examples in ?fitme, ?corrHLfit, ?Loaloa, or ?arabidopsis;
# see examples in ?Matern for group-specific spatial effects.
       Hierachical GLMs with non-gaussian random effects
data("salamander")
if (spaMM.getOption("example_maxtime")>1) {
 # both gaussian and non-gaussian random effects
 fitme(cbind(Mate,1-Mate)~1+(1|Female)+(1|Male),family=binomial(),
        rand.family=list(gaussian(),Beta(logit)),data=salamander)
 # Random effect of Male nested in that of Female:
 fitme(cbind(Mate,1-Mate)~1+(1|Female/Male),
       family=binomial(),rand.family=Beta(logit),data=salamander)
# [ also allowed is cbind(Mate,1-Mate)~1+(1|Female)+(1|Male %in% Female) ]
}
##
      Modelling residual variance ( = structured-dispersion models)
# GLM response, fixed effects for residual variance
fitme(y \sim 1, family=Gamma(log),
      resid.model = ~ X3+I(X3^2) ,data=wafers)
# GLMM response, and mixed effects for residual variance
if (spaMM.getOption("example_maxtime")>1.5) {
 fitme(y \sim 1+(1|batch), family=Gamma(log),
        resid.model = \sim 1+(1|batch) ,data=wafers)
}
```

spaMM-conventions

spaMM conventions and differences from related fitting procedures

#### **Description**

**input arguments** are generally similar to those of glm and (g)lmer, in particular for the spaMM::fitme function, with the exception of the prior.weights argument, which is simply weights in the other packages. The name prior.weights seems more consistent, since e.g. glm returns its input

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weights as output prior.weights, while its output weights are instead the weights in the final iteration of an iteratively weighted least-square fit.

The **default likelihood target** for dispersion parameters is restricted likelihood (REML estimation) for corrHLfit and (marginal) likelihood (ML estimation) for fitme. Model fits may provide restricted likelihood values(ReL) even if restricted likelihood is is not used as an objective function at any step in the analysis.

See good-practice for advice about the proper syntax of formula.

Computation times depend on control parameters given by spaMM.getOption("spaMM\_tol") parameters (for iterative algorithms), and spaMM.getOption("nloptr") parameters for the default optimizer. Do not use spaMM.options() to control them globally, unless you know what you are doing. Rather control them locally by the control.HLfit argument to control spaMM\_tol, and by the control arguments of corrHLfit and fitme to control nloptr. If nloptr\$Xtol\_rel is set above 5e-06, fitme will by default refit the fixed effects and dispersion parameters (but not other correlation parameters estimated by nloptr) by the iterative algorithm after nloptr convergence. Increasing nloptr\$Xtol\_rel value may therefore switches the bulk of computation time from the optimizer to the iterative algorithm, and may increase or decrease computation time depending on which algorithm is faster for a given input. Use control\$refit if you wish to inhibit this, but note that by default it provides a rescue to a poor nloptr result due to a too large Xtol\_rel.

#### References

Chambers J.M. (2008) Software for data analysis: Programming with R. Springer-Verlag New York

spaMM.colors

A flashy color palette.

#### **Description**

spaMM. colors is the default color palette for some color plots in spaMM.

#### Usage

```
spaMM.colors(n = 64, redshift = 1, adjustcolor_args=NULL)
```

#### **Arguments**

n

Number of color levels returned by the function. A calling graphic function with argument nlevels will typically take the first (i.e., bluest) nlevels color levels. If n<nlevels, the color levels are recycled

redshift

The higher it is, the more the palette blushes....

adjustcolor\_args

Either NULL or a list of arguments for adjustcolor, in which case adjustcolor is called to modify spaMM.colors's default vector of colors. See the documentation of the latter function for further information. All arguments except col are possible.

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#### **Details**

If you don't like this color palette, have a look at the various ones provided by the fields package.

# Value

A vector giving the colors in a hexadecimal format.

## **Examples**

```
## see mapMM examples
```

```
spaMM.filled.contour Level (Contour) Plots with better aspect ratio control (for geographical maps, at least)
```

## Description

This function is derived from filled.contour in the graphics package, and this documentation is likewise heavily based on that of filled.contour.

This function likewise produces a contour plot with the areas between the contours filled in solid color, and a key showing how the colors map to z values is likewise shown to the right of the plot. The only difference is the way the aspect ratio is determined and can be controlled (using the map. asp parameter instead of asp), They thus easily provide nice-looking maps with meaningful latitude/longitude ratio (see Examples). However, this does not work well with rstudio.

# Usage

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# Arguments

x, y	locations of grid lines at which the values in z are measured. These must be in ascending order. (The rest of this description does not apply to .filled.contour.) By default, equally spaced values from 0 to 1 are used. If x is a list, its components x\$x and x\$y are used for x and y, respectively. If the list has component z this is used for z.
Z	a numeric matrix containing the values to be plotted Note that x can be used instead of z for convenience.
xrange	x range of the plot.
yrange	y range of the plot.
zrange	z range of the plot.
margin	This controls how far (in relative terms) the plot extends beyond the x and y ranges of the analyzed points, and is overriden by explicit xrange and yrange arguments.
levels	a set of levels which are used to partition the range of z. Must be <b>strictly</b> increasing (and finite). Areas with z values between consecutive levels are painted with the same color.
nlevels	if levels is not specified, the range of z, values is divided into approximately this many levels.
color.palette	a color palette function to be used to assign colors in the plot.
col	an explicit set of colors to be used in the plot. This argument overrides any palette function specification. There should be one less color than levels
plot.title	statements which add titles to the main plot.
plot.axes	statements which draw axes (and a box) on the main plot. This overrides the default axes.
key.title	
kov avos	statements which add titles for the plot key.
key.axes	statements which add titles for the plot key. statements which draw axes on the plot key. This overrides the default axis.
map.asp	·
•	statements which draw axes on the plot key. This overrides the default axis. the y/x aspect ratio of the 2D plot area (not of the full figure including the scale).
map.asp	statements which draw axes on the plot key. This overrides the default axis. the y/x aspect ratio of the 2D plot area (not of the full figure including the scale). Default is (plotted y range)/(plotted x range) (i.e., scales for x are identical).
map.asp xaxs	statements which draw axes on the plot key. This overrides the default axis. the y/x aspect ratio of the 2D plot area (not of the full figure including the scale). Default is (plotted y range)/(plotted x range) (i.e., scales for x are identical). the x axis style. The default is to use internal labeling.
map.asp xaxs yaxs	statements which draw axes on the plot key. This overrides the default axis. the y/x aspect ratio of the 2D plot area (not of the full figure including the scale). Default is (plotted y range)/(plotted x range) (i.e., scales for x are identical). the x axis style. The default is to use internal labeling. the y axis style. The default is to use internal labeling. the style of labeling to be used. The default is to use horizontal labeling.
map.asp  xaxs  yaxs  las	statements which draw axes on the plot key. This overrides the default axis. the y/x aspect ratio of the 2D plot area (not of the full figure including the scale). Default is (plotted y range)/(plotted x range) (i.e., scales for x are identical). the x axis style. The default is to use internal labeling. the y axis style. The default is to use internal labeling. the style of labeling to be used. The default is to use horizontal labeling.

# **Details**

The values to be plotted can contain NAs. Rectangles with two or more corner values are NA are omitted entirely: where there is a single NA value the triangle opposite the NA is omitted.

Values to be plotted can be infinite: the effect is similar to that described for NA values.

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#### Value

This returns invisibly a list with elements of the plot, the x, y, z coordinates and the contour levels.

#### Note

Builds heavily on filled.contour by Ross Ihaka and R-core. spaMM.filled.contour uses the layout function and so is restricted to a full page display.

The output produced by spaMM. filled.contour is actually a combination of two plots; one is the filled contour and one is the legend. Two separate coordinate systems are set up for these two plots, but they are only used internally – once the function has returned these coordinate systems are lost. If you want to annotate the main contour plot, for example to add points, you can specify graphics commands in the plot.axes argument. See the Examples.

#### References

Cleveland, W. S. (1993) Visualizing Data. Summit, New Jersey: Hobart.

#### See Also

contour, image, palette; contourplot and levelplot from package lattice.

## **Examples**

```
spaMM.filled.contour(volcano, color.palette = spaMM.colors) # simple
## Comparing the layout with that of filled.contour:
# (except that it does not always achieve the intended effect
# in RStudio Plots pane).
x <- 10*1:nrow(volcano)
y <- 10*1:ncol(volcano)
spaMM.filled.contour(x, y, volcano, color.palette = terrain.colors,
    plot.title = title(main = "The Topography of Maunga Whau",
    xlab = "Meters North", ylab = "Meters West"),
    plot.axes = \{ axis(1, seq(100, 800, by = 100)) \}
                  axis(2, seq(100, 600, by = 100)) },
    key.title = title(main = "Height\n(meters)"),
    key.axes = axis(4, seq(90, 190, by = 10))) # maybe also asp = 1
mtext(paste("spaMM.filled.contour(.) from", R.version.string),
      side = 1, line = 4, adj = 1, cex = .66)
## compare with
filled.contour(x, y, volcano, color.palette = terrain.colors,
    plot.title = title(main = "The Topography of Maunga Whau",
    xlab = "Meters North", ylab = "Meters West"),
    plot.axes = { axis(1, seq(100, 800, by = 100))
                  axis(2, seq(100, 600, by = 100)) },
    key.title = title(main = "Height\n(meters)"),
    key.axes = axis(4, seq(90, 190, by = 10))) # maybe also asp = 1
mtext(paste("filled.contour(.) from", R.version.string),
```

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```
side = 1, line = 4, adj = 1, cex = .66)
```

spaMM\_boot

Parametric bootstrap

## **Description**

spaMM\_boot simulates samples from a fit object inheriting from class "HLfit", as produced by spaMM's fitting functions, and applies a given function to each simulated sample. Parallelization is supported (see Details).

spaMM2boot is similar except that it assumes that the original model is refitted on the simulated data, and the given function is applied to the refitted model, and the value is in a format directly usable as input for boot::boot.ci.

Both of these functions can be used to apply standard parametric bootstrap procedures. spaMM\_boot is suitable for more diverse applications, e.g. to fit by one model some samples simulated under another model (see Example).

# Usage

```
spaMM_boot(object, simuland, nsim, nb_cores=NULL, seed=NULL,
           resp_testfn=NULL, control.foreach=list(),
           debug. = FALSE, type, fit_env=NULL, cluster_args=NULL,
           showpbar= eval(spaMM.getOption("barstyle")),
          boot_samples=NULL,
           ...)
spaMM2boot(object, statFUN, nsim, nb_cores=NULL, seed=NULL,
           resp_testfn=NULL, control.foreach=list(),
           debug. = FALSE, type="marginal", fit_env=NULL,
           cluster_args=NULL, showpbar= eval(spaMM.getOption("barstyle")),
           boot_samples=NULL,
           ...)
```

# **Arguments**

object	The fit object to simulate from.
simuland	The function to apply to each simulated sample. See Details for requirements of this function.
statFUN	The function to apply to each fit object for each simulated sample. See Details for requirements of this function.
nsim	Number of samples to simulate and analyze.
nb_cores	Number of cores to use for parallel computation. The default is spaMM.getOption("nb_cores"), and 1 if the latter is NULL.nb_cores=1 prevents the use of parallelisation procedures.
seed	Passed to simulate.HLfit

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resp\_testfn

Passed to simulate. HLfit; NULL, or a function that tests a condition which simulated samples should satisfy. This function takes a response vector as argument and return a boolean (TRUE indicating that the sample satisfies the condition).

control.foreach

list of control arguments for foreach. These include in particular .combine (with default value "rbind"), and .errorhandling (with default value "remove", but "pass" is quite useful for debugging).

debug.

Boolean (or integer, interpreted as boolean). For debugging purposes, given that spaMM\_boot does not stop when the fit of a bootstrap replicate fails. Subject to changes with no or little notice. In serial computation, debug.=2 will stop on an error. In parallel computation, this would be ignored. The effect of debug.=TRUE depends on what simuland does of it. The default simuland for likelihood ratio testing functions, eval\_replicate, shows how debug. can be used to control a call to dump.frames (however, debugging user-defined functions by such a call does not require control by debug.).

type

Character: passed to simulate. HLfit. Defaults, with a warning, to type="marginal" in order to replicate the behaviour of previous versions of spaMM\_boot. This is an appropriate default for various parametric bootstrpa analyses, but not necessarily the appropriate type for all possible uses. See Details of simulate. HLfit for other implemented options.

fit\_env

An environment or list containing variables necessary to evaluate simuland on each sample, and not included in the fit object. E.g., use fit\_env=list(phi\_fix=phi\_fix) if the fit assumed fixed=list(phi=phi\_fix): the name in list(phi\_fix=<.>) must be the name of the object that will be sought by the called process when interpreting fixed=list(phi=phi\_fix) (if still unsure about the proper syntax, see the clusterExport documentation, as fit\_env is used in the following context: parallel::clusterExport(cl=<cluster>, varlist=ls(fit\_env), envir=fit\_env)).

cluster\_args

NULL or a list of arguments, passed to makeCluster.

showpbar

Controls display of progress bar. See barstyle option for details.

boot\_samples

NULL, or precomputed bootstrap samples from the fitted model, provided as a matrix with one column per bootstrap replicate (the format of the result of simulate.HLfit), or as a list including a bootreps element with the same

matrix format.

... Further arguments passed to the simuland function.

#### **Details**

The simuland function must take as first argument a vector of response values, and may have other arguments including '...'. When required, these additional arguments must be passed through the '...' arguments of spaMM\_boot. Variables needed to evaluate them must be available from within the simuland function or otherwise provided as elements of fit\_env.

The statFUN function must take as first argument (named refit) a fit object, and may have other arguments including '...' handled as for simuland.

spaMM\_boot handles parallel backends with different features. pbapply::pbapply has a very simple interface (essentially equivalent to apply) and provides progress bars, but (in version 1.4.0,

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at least) does not have efficient load-balancing. doSNOW also provides a progress bar and allows more efficient load-balancing, but its requires foreach. foreach handles errors differently from pbapply (which will simply stop if fitting a model to a bootstrap replicate fails): see the foreach documentation.

spaMM\_boot calls simulate.HLfit on the fit object and applies simuland on each column of the matrix returned by this call. simulate.HLfit uses the type argument, which must be explicitly provided.

#### Value

spaMM\_boot returns a list, with the following element(s) (unless debug. is TRUE):

**bootreps** nsim return values in the format returned either by apply or parallel::parApply or by foreach::`%dopar%` as controlled by control.foreach\$.combine (which is here "rbind" by default).

**RNGstate** (absent in the case the boot\_samples argument was used to provide the new response values but not the RNGstate) the state of .Random. seed at the beginning of the sample simulation.

spaMM2boot returns a list suitable for use by boot.ci, with elements:

t nsim return values of the simulated statistic (in matrix format).

to nsim return the value of statFUN from the original fit.

**sim** The simulation type ("parametric").

R nsim

**.Random.seed** the state of .Random. seed at the beginning of the sample simulation.

(other elements of an object of class boot are currently not included.)

# **Examples**

```
if (spaMM.getOption("example_maxtime")>7) {
data("blackcap")
# Generate fits of null and full models:
lrt <- fixedLRT(null.formula=migStatus ~ 1 + Matern(1|longitude+latitude),</pre>
                 formula=migStatus ~ means + Matern(1|longitude+latitude),
                 method='ML',data=blackcap)
# The 'simuland' argument:
myfun <- function(y, what=NULL, lrt, ...) {</pre>
   data <- lrt$fullfit$data</pre>
  data$migStatus <- y ## replaces original response (! more complicated for binomial fits)
    full_call <- getCall(lrt$fullfit) ## call for full fit</pre>
    full_call$data <- data
    res <- eval(full_call) ## fits the full model on the simulated response
   if (!is.null(what)) res <- eval(what)(res=res) ## post-process the fit</pre>
   return(res) ## the fit, or anything produced by evaluating 'what'
 # where the 'what' argument (not required) of myfun() allows one to control
```

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```
# what the function returns without redefining the function.
 # Call myfun() with no 'what' argument: returns a list of fits
 spaMM_boot(lrt$nullfit, simuland = myfun, nsim=1, lrt=lrt,
             type ="marginal")[["bootreps"]]
 # Return only a model coefficient for each fit:
 spaMM_boot(lrt$nullfit, simuland = myfun, nsim=7,
             what=quote(function(res) fixef(res)[2L]),
             lrt=lrt, type ="marginal")[["bootreps"]]
 ## Not run:
    # Parametric bootstrap by spaMM2boot() and spaMM_boot():
    boot.ci_info <- spaMM2boot(lrt$nullfit, statFUN = function(refit) fixef(refit)[1],</pre>
                                nsim=99, type ="marginal")
    boot::boot.ci(boot.ci_info, , type=c("basic","perc","norm"))
    nullfit <- lrt$nullfit</pre>
    boot_t <- spaMM_boot(lrt$nullfit, simuland = function(y, nullfit) {</pre>
      refit <- update_resp(nullfit, y)</pre>
      fixef(refit)[1]
    }, nsim=99, type ="marginal", nullfit=nullfit)$bootreps
    boot::boot.ci(list(R = length(boot\_t), sim="parametric"), t0=fixef(nullfit)[1],\\
                  t= t(boot_t), type=c("basic","perc","norm"))
## End(Not run)
```

spaMM\_glm.fit

Fitting generalized linear models without initial-value or divergence headaches

# Description

spaMM\_glm.fit is a stand-in replacement for glm.fit, which can be called through glm by using glm(<>, method="spaMM\_glm.fit"). Input and output structure are exactly as for glm.fit. It uses a Levenberg-Marquardt algorithm to prevent divergence of estimates. For models families such as Gamma() (with default inverse link) where the linear predictor is constrained to be positive, if the **rcdd** package is installed, the function can automatically find valid starting values or else indicate that no parameter value is feasible. It also automatically provides good starting values in some cases where the base functions request them from the user (notably, for gaussian(log) with some negative response). spaMM\_glm is a convenient wrapper, calling glm with default method glm.fit, then calling method spaMM\_glm.fit, with possibly different initial values, if glm.fit failed.

## Usage

```
spaMM_glm.fit(x, y, weights = rep(1, nobs), start = NULL, etastart = NULL,
```

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## **Arguments**

All arguments except strict are common to these functions and their stats package equivalents, glm and glm.fit. Most arguments operate as for the latter functions, whose documentation is repeated below. The control argument may operate differently.

formula	an object of class "formula" (or one that can be coerced to that class): a sym-
	bolic description of the model to be fitted. The details of model specification are

given in the 'Details' section of glm.

family a description of the error distribution and link function to be used in the model.

For spaMM\_glm this can be a character string naming a family function, a family function or the result of a call to a family function. For spaMM\_glm.fit only the

third option is supported. (See family for details of family functions.)

data an optional data frame, list or environment (or object coercible by as.data.frame

to a data frame) containing the variables in the model. If not found in data, the variables are taken from environment(formula), typically the environment

from which glm is called.

weights an optional vector of 'prior weights' to be used in the fitting process. Should be

NULL or a numeric vector.

subset an optional vector specifying a subset of observations to be used in the fitting

process.

na.action a function which indicates what should happen when the data contain NAs. The

default is set by the na.action setting of options, and is na.fail if that is unset. The 'factory-fresh' default is na.omit. Another possible value is NULL,

no action. Value na. exclude can be useful.

start starting values for the parameters in the linear predictor.

etastart starting values for the linear predictor.
mustart starting values for the vector of means.

offset this can be used to specify an a priori known component to be included in the

linear predictor during fitting. This should be NULL or a numeric vector of length equal to the number of cases. One or more offset terms can be included in the formula instead or as well, and if more than one is specified their sum is used.

See model.offset.

control a list of parameters for controlling the fitting process. This is passed to glm. control,

as for glm.fit. Because one can assume that spaMM\_glm.fit will converge in many cases where glm.fit does not, spaMM\_glm.fit allows more iterations (200) by default. However, if spaMM\_glm.fit is called through glm(. . ., method="spaMM\_glm.fit"), then the number of iterations is controlled by the glm.control call within glm, so that it is 25 by default, overriding the

spaMM\_glm.fit default.

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model	a logical value indicating whether <i>model frame</i> should be included as a component of the returned value.
method	A 2-elements vector specifying first the method to be used by spaMM_glm in the first attempt to fit the model, second the method to be used in a second attempt if the first failed. Possible methods include those shown in the default, "model.frame", which returns the model frame and does no fitting, or user-supplied fitting functions. These functions can be supplied either as a function or a character string naming a function, with a function which takes the same arguments as glm.fit.
x, y	For $pam_glm$ : x is a design matrix of dimension $n * p$ , and y is a vector of observations of length n.
	For $pamM_glm.fit: x is a design matrix of dimension n * p, and y is a vector of observations of length n.$
singular.ok	logical; if FALSE a singular fit is an error.
contrasts	an optional list. See the contrasts.arg of model.matrix.default.
intercept	logical. Should an intercept be included in the <i>null</i> model?
strict	logical. Whether to perform a fit by spaMM_glm.fit if glm.fit returned the warning "glm.fit: algorithm did not converge".
• • •	arguments to be used to form the default control argument if it is not supplied directly.

# Value

An object inheriting from class glm. See glm for details.

## Note

The source and documentation is derived in large part from those of glm.fit.

# Examples

```
x <- c(8.752,20.27,24.71,32.88,27.27,19.09)
y <- c(5254,35.92,84.14,641.8,1.21,47.2)

# glm(.) fails:
(check_error <- try(glm(y~ x,data=data.frame(x,y),family=Gamma(log)), silent=TRUE))
if ( ! inherits(check_error,"try-error")) stop("glm(.) call unexpectedly succeeded")

spaMM_glm(y~ x,data=data.frame(x,y),family=Gamma(log))

## Gamma(inverse) examples
x <- c(43.6,46.5,21.7,18.6,17.3,16.7)
y <- c(2420,708,39.6,16.7,46.7,10.8)

# glm(.) fails (can't find starting value)
(check_error <- suppressWarnings(try(glm(y~ x,data=data.frame(x,y),family=Gamma()), silent=TRUE)))
if ( ! inherits(check_error,"try-error")) stop("glm(.) call unexpectedly succeeded.")</pre>
```

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```
if (requireNamespace("rcdd",quietly=TRUE)) {
    spaMM_glm(y~ x,data=data.frame(x,y),family=Gamma())
}

## A simple exponential regression with some negative response values

set.seed(123)
x <- seq(50)
y <- exp( -0.1 * x) + rnorm(50, sd = 0.1)
glm(y~ x,data=data.frame(x,y),family=gaussian(log), method="spaMM_glm.fit")

# => without the 'method' argument, stats::gaussian(log)$initialize() is called
# and stops on negative response values.
```

stripHLfit

Reduce the size of fitted objects

# **Description**

Large matrices and other memory-expensive objects may be stored in a fit object. This function removes them in order to reduce the size of the object, particularly when stored on disk. In principle, the removed objects can be regenerated automatically when needed (e.g., for a predict()).

# Usage

```
stripHLfit(object, ...)
```

# **Arguments**

object The result of a fit (an object of class HLfit).

... Further arguments, not currently used.

## Value

The input fit objects with some elements removed.

#### Note

The effect may change without notice between versions as the efficiency of the operation is highly sensitive to implementation details.

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## **Examples**

```
## Not run:
## rather unconvincing example : quantitative effect is small.
# measure size of saved object:
saveSize <- function (object,...) {</pre>
    tf <- tempfile(fileext = ".RData")</pre>
    on.exit(unlink(tf))
    save(object, file = tf,...)
    file.size(tf)
 }
data("Loaloa")
lfit <- fitme(cbind(npos,ntot-npos)~elev1+elev2+elev3+elev4+maxNDVI1+seNDVI</pre>
                    +Matern(1|longitude+latitude), method="HL(0,1)",
               data=Loaloa, family=binomial(), fixed=list(nu=0.5,rho=1,lambda=0.5))
saveSize(lfit)
pfit <- predict(lfit,newdata=Loaloa,variances=list(cov=TRUE)) # increases size!</pre>
saveSize(lfit)
lfit <- stripHLfit(lfit)</pre>
saveSize(lfit)
## End(Not run)
```

summary.HLfit

Summary and print methods for fit and test results.

# **Description**

Summary and print methods for results from HLfit or related functions. summary may also be used as an extractor (see e.g. beta\_table).

# Usage

```
## S3 method for class 'HLfit'
summary(object, details=FALSE, max.print=100L, verbose=TRUE, ...)
## S3 method for class 'HLfitlist'
summary(object, ...)
## S3 method for class 'fixedLRT'
summary(object, verbose=TRUE, ...)
## S3 method for class 'HLfit'
print(x,...)
## S3 method for class 'HLfitlist'
print(x,...)
## S3 method for class 'fixedLRT'
print(x,...)
```

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# Arguments

object An object of class HLfit, as returned by the fitting functions in spaMM.

x The return object of HLfit or related functions.

verbose For summary. HLfit, whether to print the screen output that is the primary pur-

pose of summary. verbose=FALSE may be convenient when summary is used as an extractor. For summary.fixedLRT, whether to print the model fits or not.

max.print Controls options("max.print") locally.

details A vector with elements controlling whether to print some obscure details. El-

ement ranCoefs=TRUE will print details about random-coefficients terms (see Details); and element p\_value="Wald" will print a p-value for the t-value of each fixed-effect coefficient, assuming a gaussian distribution of the test statistic (but, beyond the generally questionable nature of p-value tables, see e.g. LRT

and fixedLRT for alternative testing approaches).

... further arguments passed to or from other methods.

#### **Details**

The random effect terms of the linear predictor are of the form  $\mathbf{ZLv}$ . In particular, for  $\mathbf{random-coefficients}$  models (i.e., including random-effect terms such as  $(\mathsf{z}|\mathsf{group})$  specifying a random-slope component), correlated random effects are represented as  $\mathbf{b} = \mathbf{Lv}$  for some matrix  $\mathbf{L}$ , and where the elements of  $\mathbf{v}$  are uncorrelated. In the output of the fit, the  $\mathsf{Var}$ . column gives the variances of the correlated effects,  $\mathbf{b} = \mathbf{Lv}$ . The  $\mathsf{Corr}$ . column(s) give their correlation(s). If details is TRUE, estimates and SEs of the (log) variances of the elements of  $\mathbf{v}$  are reported as for other random effects in the  $\mathsf{Estimate}$  and  $\mathsf{cond}$ . SE. columns of the table of lambda coefficients. However, this non-default output is potentially misleading as the elements of  $\mathbf{v}$  cannot generally be assigned to specific terms (such as intercept and slope) of the random-effect formula, and the representation of  $\mathbf{b}$  as  $\mathsf{Lv}$  is not unique.

## Value

The return value is a list whose elements may be subject to changes, but two of them can be considered stable, and are thus part of the API: the beta\_table and lambda\_table which are the displayed tables for the coefficients of fixed effects and random-effect variances.

#### **Examples**

## see examples of fitme() or corrHLfit() usage

update.HLfit Updates a fit

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## **Description**

update and update\_resp will update and (by default) re-fit a model. They do this mostly by extracting the call stored in the object, updating the call and evaluating that call. Using update(<fit>) is a risky programming style (see Details). update\_formulas(<mv fit>, ...) can update formulas from a fitmv fit as well as the single formula of a fit by the other fitting functions.

update\_resp handles a new response vector as produced by simulate.

#### Usage

```
## S3 method for class 'HLfit'
update(object, formula., ..., evaluate = TRUE)
update_resp(object, newresp, ..., evaluate = TRUE)

update_formulas(object, formula., ...)

# <fit object>$respName[s] : see Details.
```

## Arguments

object A return object from an HLfit call.

formula. A standard formula; or a formula with a peculiar syntax only describing changes

to the original model formula (see update. formula for details); or (for multivariate-

response models) a list of formula of such types.

newresp New response vector.

... Additional arguments to the call, or arguments with changed values. Use *name* 

= NULL to remove the argument with given *name*.

evaluate If TRUE, evaluate the new call else return the call.

## **Details**

Controlling response updating: Updating the data may be tricky when the response specified in a formula is not simply the name of a variable in the data. For example, if the response was specified as I(foo^2) the variable foo is not what simulate. HLfit will simulate, so foo should not be updated with such simulation results, yet this is what should be updated in the data. For some time **spaMM** has handled such cases by using an alternative way to provide updated response information, but this has some limitations. So **spaMM** now update the data after checking that this is correct, which the consequence that when response updating is needed (notably, for bootstrap procedures), the response should preferably be specified as the name of a variable in the data, rather than a more complicated expression.

However, in some cases, dynamic evaluation of the response variable may be helpful. For example, for bootstrapping hurdle models, the zero-truncated response may be specified as I(count[presence>0] <- NA; count) (where both the zero-truncated count and binary presence variables are both updated by the bootstrap simulation). In that case the names of the two variables to be updated is provided by setting (say)

```
<fit object>$respNames <- c("presence", "count")</pre>
```

for an hurdle model fit as a bivariate-response model, with first submodel for presence/absence, and

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second submodel for zero-truncated response. A full example is developed in the "Gentle introduction" to **spaMM** (https://gitlab.mbb.univ-montp2.fr/francois/spamm-ref/-/blob/master/vignettePlus/spaMMintro.pdf). Alternatively for univariate-response fits, use <fit object>\$respName <- "count"

Controlling formula updating: Early versions of spaMM's update method relied on stats::update.formula whose results endorse stats's (sometimes annoying) convention that a formula without an explicit intercept term actually includes an intercept. spaMM::update.HLfit was then defined to avoid this problem. Formula updates should still be carefully checked, as getting them perfect has not been on the priority list.

Various post-fit functions from base R may use update.formula directly, rather than using automatic method selection for update.update.formula is not itself a generic, which leads to the following problem. To make update.formula() work on multivariate-response fits, one would like to be able to redefine it as a generic, with an HLfit method that would perform what update\_formulas does, but such a redefinition appears to be forbidden in a package distributed on CRAN. Instead it is suggested to define a new generic spaMM::update, which could have a spaMM::update.formula as a method (possibly itself a generic). This would be of limited interest as the new spaMM::update.formula would be visible to spaMM::update but not to stats::update, and thus the post-fit functions from base R would still not use this method.

**Safe updating**: update(<fit>, ...), as a general rule, is tricky. update methods are easily affected in a non-transparent way by changes in variables used in the original call. For example

```
foo <- rep(1,10)
m <- lm(rnorm(10)~1, weights=foo)
rm(foo)
update(m, .~.) # Error</pre>
```

To avoid such problems, **spaMM** tries to avoid references to variables in the global environment, by enforcing that the data are explicitly provided to the fitting functions by the data argument, and that any variable used in the prior.weights argument is in the data.

Bugs can also result when calling update on a fit produced within some function, say function somefn calling fitme(data=mydata,...), as e.g. update(<fit>) will then seek a global variable mydata that may differ from the fitted mydata which was local to somefn.

#### Value

update.formula(object) returns an object of the same nature as formula(object). The other functions and methods return an HLfit fit of the same type as the input object, or a call object, depending on the evaluate value. **Warning:** The object returned by update\_resp cannot be used safely for further programming, for the reason explained in the Details section.

## See Also

```
See also HLCor, HLfit.
```

# **Examples**

```
data("wafers")
## First the fit to be updated:
```

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```
wFit <- HLfit(y \sim X1 \times X3 + X2 \times X3 + I(X2^2) + (1|batch), family=Gamma(log),
          resid.model = \sim X3+I(X3^2) ,data=wafers)
newresp <- simulate(wFit)</pre>
update_resp(wFit,newresp=newresp)
# For estimates given by Lee et al., Appl. Stochastic Models Bus. Ind. (2011) 27: 315-328:
# Refit with given beta or/and phi values:
betavals < c(5.55, 0.08, -0.14, -0.21, -0.08, -0.09, -0.09)
# reconstruct fitted phi value from predictor for log(phi)
Xphi <- with(wafers,cbind(1,X3,X3^2)) ## design matrix</pre>
phifit \leftarrow exp(Xphi %*% c(-2.90,0.1,0.95))
upd_wafers <- wafers
designX <- get_matrix(wFit)</pre>
upd_wafers$off_b <- designX %*% betavals
update(wFit,formula.= . ~ offset(off_b)+(1|batch), data=upd_wafers,
       ranFix=list(lambda=exp(-3.67),phi=phifit))
## There are subtlety in performing REML fits of constrained models,
    illustrated by the fact that the following fit does not recover
     the original likelihood values, because dispersion parameters are
     estimated but the REML correction changes with the formula:
upd_wafers$off_f <- designX %*% fixef(wFit) ## = predict(wFit,re.form=NA,type="link")
update(wFit,formula.= . ~ offset(off_f)+(1|batch), data=upd_wafers)
## To maintain the original REML correction, Consider instead
update(wFit,formula.= . \sim offset(off_f)+(1|batch), data=upd_wafers,
       REMLformula=formula(wFit)) ## recover original p_v and p_bv
## Alternatively, show original wFit as differences from betavals:
update(wFit,formula.= . ~ . +offset(off_f), data=upd_wafers)
```

vcov

Extract covariance or correlation components from a fitted model object

# **Description**

summary(<fit object>)\$beta\_table returns the table of fixed-effect coefficients as it is printed by summary, including standard errors and t-values.

vcov returns the variance-covariance matrix of the fixed-effects coefficients (cf See Also for related computations involving random effects).

Corr by default returns correlation matrices of random effects (though see Details for user-defined correlation models).

VarCorr returns (co)variance parameters of random effects, and optionally the residual variance(s), from a fit object, in a data frame format roughly consistent with the method of objects of class "lme", in particular including columns with consistent names for easier extraction. One may have to consult the summary of the object to check the meaning of the contents of this data frame

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(e.g., of 'variance' coefficients for non-gaussian random effects). Other extractors to consider are get\_ranPars and get\_inits\_from\_fit, the latter providing parameters in a form suitable for initializing a fit.

The covariance matrix of residuals of a fit can be obtained as a block of the hat matrix (get\_matrix(., which="hat\_matrix")). This is (as other covariances matrices above) a matrix of expected values, generally assuming that the fitted model is correct and that its parameters are "well" estimated, and should not to be confused with the computation of diagnostic correlations among inferred residuals of a fit.

#### Usage

```
## S3 method for class 'HLfit'
vcov(object, ...)
## S3 method for class 'HLfit'
VarCorr(x, sigma = 1, add_residVars=TRUE, verbose=TRUE, ...)
Corr(object, A=TRUE, cov2cor.=TRUE, ...)
```

## **Arguments**

object, x	A fitted model object, inheriting from class "HLfit", as returned by the fitting functions in spaMM.
add_residVars	Boolean; whether to include residual variance information in the returned table.
sigma	ignored argument, included for consistency with the generic function.
A	Boolean: Whether to return the correlation matrix described by the <b>AL</b> matrix product, when there is an <b>A</b> matrix (as for IMRF terms; see random-effects).
cov2cor.	Boolean: Whether to convert covariance matrices to correlation matrices (see Details).
verbose	Boolean: Whether to print some notes.
	Other arguments that may be needed by some method.

## **Details**

Any matrix returned by the Corr extractor is by default the unconditional correlation matrix of a vector "**ALv**" of random effects (as defined in random-effects).

But it may also be an heteroscedastic matrix for some random effects if cov2cor. is set to FALSE. In particular, the IMRF and MaternIMRFa models are by default defined in terms of the inverse of an heteroscedastic covariance matrix (with tcrossprod factor L), and of a A matrix of weights. The product AL will be the tcrossprod factor of a covariance matrix rather than a correlation matrix, unless a non-default normalization was requested when declaring the random-effect terms. User-defined random-effects models may also be heteroscedastic. In all these cases Corr will by default return the correlation matrix, by applying cov2cor to the tcrossproduct.

#### Value

vcov returns a matrix.

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Corr returns a list, for the different random effect terms. For each random-effect term with nontrivial correlation structure, the returned element is a matrix, returned in base matrix format or in some class from **Matrix**. Otherwise the it is an information message.

VarCorr returns either NULL (if no variance to report, as for a poisson GLM) or a data frame with columns for the grouping factor, term, variance of random effect, standard deviation (the root of the variance), and optionally for correlation of random effect in random-coefficient terms. Information about the residual variance is optionally included as the last row(s) of the data frame, when relevant (gaussian- or Gamma-response models with single scalar parameter; beware the meaning of the residual variance parameter for Gamma-response models).

Some variance parameters may be removed from the VarCorr output, with a message, such as the slope of the linear predictor describing the correlation model of an adjacency term (see autoregressive). The rare user of such parametrization should not consider this as a stable feature.

#### See Also

```
get_inits_from_fit and get_ranPars.
```

get\_matrix(., which="beta\_v\_cov") for the joint covariance matrix of estimates/predictions of fixed-effect coefficients and random effects; and

get\_matrix(., which="v\_condcov") for the covariance matrix of predictions of random effects given fixed effects (the variances corresponding to the condsd reported in some **lme4** output). Both of these computations refer to the random effects **v** as defined in random-effects.

## **Examples**

```
data("wafers")
m1 <- HLfit(y ~ X1+X2+(1|batch), resid.model = ~ 1 ,data=wafers, method="ML")
vcov(m1)

# Example from VarCorr() documentation in 'nlme' package
data("Orthodont",package = "nlme")
sp1 <- fitme(distance ~ age+(age|Subject), data = Orthodont, method="REML")
VarCorr(sp1)</pre>
```

verbose

Tracking progress of fits

## **Description**

This (partially) documents the usage of the verbose argument of the fitting functions, and more specifically of verbose["TRACE"] values.

Default is TRACE=FALSE (or 0) which is self-explanatory. TRACE=TRUE (or 1) shows values of outer-estimated parameters (and possibly fixed values of parameters that would be outer-estimated), some cryptic progress bar, and the attained value of the likelihood objective function (but when there inner-estimated dispersion parameters, the output is more difficult to describe concisely). Other values have effect may change in later versions without notice see Details).

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If the fitted model includes a residual-dispersion mdoel, some tracing output for the latter may be confusingly intermingled with tracing output of the mean-response model. The Details are valid only for the mean-response model.

#### **Details**

0<TRACE<1 only shows the cryptic progress bar.

TRACE=2 will further show information about the progress of Levenberg-Marquardt-like steps for linear-predictor coefficients.

TRACE=3 will further show information about the progress of distinct Levenberg-Marquardt-like steps random effects given fixed-effect coefficients.

TRACE=4 will further show cryptic information about which matrix computations are requested.

TRACE=5 will further report (through a call to the base trace function) the str(.) of the results of such matrix computations.

TRACE=6 will further pause between iterations of the reweighted least-squares algorithm, allowing a browser session to be called.

wafers

Data from a resistivity experiment for semiconductor materials.

# Description

This data set was reported and analyzed by Robinson et al. (2006) and reanalyzed by Lee et al. (2011). The data "deal with wafers in a single etching process in semiconductor manufacturing. Wafers vary through time since there are some variables that are not perfectly controllable in the etching process. For this reason, wafers produced on any given day (batch) may be different from those produced on another day (batch). To measure variation over batch, wafers are tested by choosing several days at random. In this data, resistivity is the response of interest. There are three variables, gas flow rate (x1), temperature (x2), and pressure (x3) and one random effect (batch or day)." (Lee et al 2011).

## Usage

```
data("wafers")
```

# **Format**

The data frame includes 198 observations on the following variables:

**y** resistivity.

batch batch, indeed.

X1 gas flow rate.

X2 temperature.

X3 pressure.

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# **Source**

This data set was manually pasted from Table 3 of Lee et al. (2011). Transcription errors may have occurred.

#### References

Robinson TJ, Wulff SS, Montgomery DC, Khuri AI. 2006. Robust parameter design using generalized linear mixed models. Journal of Quality Technology 38: 38–65.

Lee, Y., Nelder, J.A., and Park, H. 2011. HGLMs for quality improvement. Applied Stochastic Models in Business and Industry 27, 315-328.

# **Examples**

## see examples in the main Documentation page for the package.

welding

Welding data set

# Description

The data give the results of an unreplicated experiment for factors affecting welding quality conducted by the National Railway Corporation of Japan (Taguchi and Wu, 1980, cited in Smyth et al., 2001). It is a toy example for heteroscedastic models and is also suitable for illustrating fit of overparameterized models.

#### Usage

```
data("welding")
```

#### **Format**

The data frame includes 16 observations on 10 variables:

**Strengh** response variable;

... nine two-level factors.

#### Source

The data were downloaded from http://www.statsci.org/data/general/welding.txt on 2014/08/19 and are consistent with those shown in table 5 of Bergman and Hynén (1997).

## References

Bergman B, Hynén A (1997) Dispersion effects from unreplicated designs in the  $2^{k-p}$  series. Technometrics, 39, 191–98.

Smyth GK, Huele AF, Verbyla AP (2001). Exact and approximate REML for heteroscedastic regression. Statistical Modelling 1, 161-175.

Taguchi G, Wu Y (1980) Introduction to off-line quality control. Nagoya, Japan: Central Japan Quality Control Association.

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## **Examples**

```
data("welding")
## toy example from Smyth et al.
fitme(Strength ~ Drying + Material, resid.model = ~ Material+Preheating ,data=welding, method="REML")
## toy example of overparameterized model
fitme(Strength ~ Rods+Thickness*Angle+(1|Rods), resid.model = ~ Rods+Thickness*Angle ,data=welding)
```

WinterWheat

Example of yield stability analysis

# **Description**

Translation of an example that may be found at

https://www.r-bloggers.com/2019/06/genotype-experiments-fitting-a-stability-variance-model-with-r/based on yield of eight durum wheat genotypes over seven years, following a randomised block design with three replicates. A genotype-in-year random effect is used to quantify genotype-by-environment interactions. In the first fit (constvar), the variance of this random effect is constant over genotypes. In the second fit (varvar), different variances are fitted for the distinct genotypes, to assess the relative stability of yield of the different genotypes over environments. This second model can be fitted as a constrained random-coefficient model, where the constraint describes a diagonal covariance matrix for the random coefficients.

This example uses the fact that the argument fixed=list(ranCoefs=<...>) can be used to fit a covariance matrix with an arbitrary set of constrained elements. Only elements left as 'NA' (here the diagonal elements of the matrix) are fitted.

## **Examples**

```
if (spaMM.getOption("example_maxtime")>1.5 &&
      requireNamespace("agridat", quietly = TRUE)) {
data("onofri.winterwheat", package="agridat")
(constvar <- fitme(</pre>
 yield \sim gen + (1|year) + (1|block %in% year)+(1|gen %in% year),
 data=onofri.winterwheat, method="REML"))
# Diagonal matrix of NA's, represented as vector for its lower triangle:
ranCoefs_for_diag <- function(nlevels) {</pre>
## Conceptual version
# diagmat <- matrix(NA, ncol=nlevels,nrow=nlevels)</pre>
# diagmat[lower.tri(diagmat,diag=FALSE)] <- 0</pre>
# return(diagmat[lower.tri(diagmat,diag=TRUE)])
## which amounts to:
vec <- rep(0,nlevels*(nlevels+1L)/2L)</pre>
vec[cumsum(c(1L,rev(seq(nlevels-1L)+1L)))] <- NA</pre>
vec
}
```

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```
(varvar <- fitme(
  yield ~ gen + (1|year) + (1|block %in% year)+(0+gen|gen %in% year), method="REML",
  data=onofri.winterwheat, fixed=list(ranCoefs=list("3"=ranCoefs_for_diag(8L)))))
}</pre>
```

wrap\_parallel

Selecting interfaces for parallelisation

# **Description**

spaMM implements three interfaces for parallelisation. Depending on their arguments, either serial computation (default), a socket cluster (parallelisation default), or a fork cluster (available in linux and alike operating systems) can be used by all interfaces.

dopar is called by default by its bootstrap procedures, and dofuture has been developed as an alternative, whose use is controlled by spaMM.options(wrap\_parallel="dofuture") (versus the default, spaMM.options(wrap\_parallel="dopar"). combinepar is the third and more recent interface; it is not a formally supported wrap\_parallel option because its additional functionalities are of no use in **spaMM**'s bootstrap procedures.

dopar is based on a patchwork of backends: for socket clusters, depending whether the **doSNOW** package is attached, foreach or pbapply is called (**doSNOW** allows more efficient load balancing than pbapply); for fork clusters, parallel::mclapply is used. This makes it impossible to ensure consistency of options across computation environments, notably of enforcing the .combine control of foreach; and this makes it error-prone to ensure identical control of random number generators in all cases (although dopar and combinepar still aim to ensure the latter control).

By contrast, dofuture is based only on the **future** and **future.apply** packages, in principle allowing a single syntax to control of random number generator across the different cases, hence repeatable results across them. This does **not** make a difference for bootstrap computations in **spaMM** as the bootstrap samples are never simulated in parallel: only refitting the models is performed in parallel, and fit results do not depend on random numbers. Further, the **future**-based code for socket clusters appears significantly slower than the one used by dopar. For these reasons, the latter function is used by default by **spaMM**.

combinepar is a third and more recent approach designed to address the other issue: it always uses **foreach** so that the .combine control is consistently enforced. It uses **future** only when no alternative is available to produce a progress bar (namely, for socket clusters when **doSNOW** is not available).

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X.GCA

Fixed-effect terms for dyadic interactions

# Description

X.GCA and X.antisym are functions which, when called in a model formula, stand for terms designed to represent the effet of symmetric interactions between pairs of individuals (order of individuals in the pair does not matter). antisym likewise represents anti-symmetric interactions (the effect of reciprocal ordered pairs on the outcome are opposite, as in the so-called Bradley-Terry models). These constructs all account for multiple membership, i.e., the fact that the same individual may act as the first or the second individual among different pairs, or even within one pair if this makes sense).

The outcome of an interaction between a pair i,j of agents is subject to a symmetric overall effect  $a_{ij}$  when the effect "on" individual i (or viewed from the perspective of individual i) equals the effect on j:  $a_{ij}=a_{ji}$ . This may result from the additive effect of individual effects  $a_i$  and  $a_j$ :  $a_{ij}=a_i+a_j$ . A X.GCA call represents such symmetric additive effects. Conversely, antisymmetry is characterized by  $a_{ij}=a_i-a_j=-a_{ji}$  and is represented by a X.antisym call. See the diallel documentation for similar constructs for random effects, for additional comments on semantics (e.g. about "GCA"), and for further references.

If individual-level factors ID1 + ID2 were included in a formula for dyadic interactions, this would result in different coefficients being fitted for the same level in each factor. By contrast, the present constucts ensure that a single coefficient is fitted for the same-named levels of factors ID1 and ID2.

# Usage

```
X.GCA(term, contr="contr.treatment", ...)
X.antisym(term, contr="contr.treatment", ...)
```

#### **Arguments**

term	an expression of the form <.>:<.> where each <.> represents a factor (or a variable that will automaticall be converted to a factor) present in the data of the fitting function call.
contr	The contrasts used. Only the default and "contr.sum" are implemented.
	For programming purposes, not documented.

#### **Details**

The fixed-effect terms (GCA(Par1,Par2), etc) from the **ImDiallel** package (Onofri & Terzaroli, 2021), defined by functions returning design matrices for usage with stats: Im, work in a formula for a **spaMM** fit, and users can define use such functions as templates for additional functions that will work similarly. However, not all post-fit functions will handle terms defined in this way well: checking robustness of predict on small and permuted newdata, as shown in the Examples, is a good test. Such problems happen because the formula-handling machinery of R handles terms represented by either a matrix or a factor, while both the model matrix and the factor information

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used to construct dyadic-interaction terms are needed to correctly predict, with new data, from models including such terms.

The presently designed functions are defined to solve this issue. By using such functions as template, users can define additional functions with the same return format (as further explained in the documented source code of X.antisym), which will allow them to perform correct predictions from fitted models.

#### Value

The functions return design matrices with additional class "factorS" and attributes "call" and "spec\_levs".

#### References

Onofri A., Terzaroli N. (2021) lmDiallel: Linear fixed effects models for diallel crosses. Version 0.9.4. https://cran.r-project.org/package=lmDiallel.

# **Examples**

```
#### Simulate dyadic data
set.seed(123)
nind <- 10
                  # Beware data grow as O(nind^2)
x <- runif(nind^2)</pre>
id12 <- expand.grid(id1=seq(nind),id2=seq(nind))</pre>
id1 <- id12$id1
id2 <- id12$id2
u \leftarrow rnorm(nind, mean = 0, sd=0.5)
## additive individual effects:
y \leftarrow 0.1 + 1*x + u[id1] + u[id2] + rnorm(nind^2, sd=0.2)
## anti-smmetric individual effects:
t < 0.1 + 1*x + u[id1] - u[id2] + rnorm(nind^2, sd=0.2)
dyaddf <- data.frame(x=x, y=y, t=t, id1=id1,id2=id2)</pre>
# : note that this contains two rows per dyad, which avoids identifiability issues.
# Enforce that interactions are between distinct individuals (not essential for the fit):
dyaddf <- dyaddf[- seg.int(1L,nind^2,nind+1L),]</pre>
# Fits:
(addfit <- fitme(y ~x +X.GCA(id1:id2), data=dyaddf))</pre>
(antifit <- fitme(t ~x +X.antisym(id1:id2), data=dyaddf))</pre>
if (FALSE) { #### check of correct handling by predict():
  # First scramble the data so that input factors are in no particular order
  set.seed(123)
```

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```
dyaddf <- dyaddf[sample(nrow(dyaddf)),]

addfiti <- fitme(y ~x +X.GCA(id1:id2), data=dyaddf)
foo <- rev(2:4)
p1 <- predict(addfiti)[foo]
p2 <- predict(addfiti, newdata=dyaddf[foo,])
diff(range(p1-p2))<1e-10  # must be TRUE
}</pre>
```

ZAXlist

S4 classes for structured matrices

# **Description**

A ZAX1ist object is a representation of the "ZAL" matrix as an S4 class holding a list of descriptors of each ZAL block for each random effect.

A Kronfacto object is a representation of a Kronecker product as an S4 class holding its factors. Methods defined for this class may avoid the computation of the Kronecker product as an actual matrix of large dimensions.

This documentation is for development purposes and may be incomplete. The objects and methods are not part of the programming interface and are subject to modification without notice.

# Usage

```
# new("ZAXlist", LIST=.)
# new("Kronfacto", BLOB=.)
```

#### **Slots**

- LIST: A list whose each element is a ZAL block represented as either a (M|m)atrix, or a list with two elements (and additional class ZA\_QCHM): ZA, and the Cholesky factor Q\_CHMfactor of the precision matrix (L=solve(Q\_CHMfactor, system="Lt")).
- BLOB: An environment holding 1hs and rhs, the factors of the Kronecker product, and other objects initialized as promises. See the source code of the non-exported .def\_Kranfacto constructor for further information.

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