# Package 'lme4'

April 3, 2018

```
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Title Linear Mixed-Effects Models using 'Eigen' and S4
Contact LME4 Authors < lme4-authors@lists.r-forge.r-project.org>
Description Fit linear and generalized linear mixed-effects models.
     The models and their components are represented using S4 classes and
     methods. The core computational algorithms are implemented using the
     'Eigen' C++ library for numerical linear algebra and 'RcppEigen' ``glue''.
Depends R (>= 3.2.0), Matrix (>= 1.2-1), methods, stats
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# Description

lme4 provides functions for fitting and analyzing mixed models: linear (lmer), generalized linear (glmer) and nonlinear (nlmer.)

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#### Differences between nlme and lme4

**lme4** covers approximately the same ground as the earlier **nlme** package. The most important differences are:

- **lme4** uses modern, efficient linear algebra methods as implemented in the Eigen package, and uses reference classes to avoid undue copying of large objects; it is therefore likely to be faster and more memory-efficient than **nlme**.
- lme4 includes generalized linear mixed model (GLMM) capabilities, via the glmer function.
- lme4 does not currently implement nlme's features for modeling heteroscedasticity and correlation of residuals.
- **lme4** does not currently offer the same flexibility as **nlme** for composing complex variance-covariance structures, but it does implement crossed random effects in a way that is both easier for the user and much faster.
- **lme4** offers built-in facilities for likelihood profiling and parametric bootstrapping.
- **lme4** is designed to be more modular than **nlme**, making it easier for downstream package developers and end-users to re-use its components for extensions of the basic mixed model framework. It also allows more flexibility for specifying different functions for optimizing over the random-effects variance-covariance parameters.
- lme4 is not (yet) as well-documented as nlme.

## Differences between current (1.0.+) and previous versions of lme4

- [gn]lmer now produces objects of class merMod rather than class mer as before
- the new version uses a combination of S3 and reference classes (see ReferenceClasses, merPredD-class, and lmResp-class) as well as S4 classes; partly for this reason it is more interoperable with nlme
- The internal structure of [gn]lmer is now more modular, allowing finer control of the different steps of argument checking; construction of design matrices and data structures; parameter estimation; and construction of the final merMod object (see modular)
- profiling and parametric bootstrapping are new in the current version
- the new version of **lme4** does *not* provide an mcmcsamp (post-hoc MCMC sampling) method, because this was deemed to be unreliable. Alternatives for computing p-values include parametric bootstrapping (bootMer) or methods implemented in the **pbkrtest** package and leveraged by the **lmerTest** package and the Anova function in the **car** package (see pvalues for more details).

## Caveats and trouble-shooting

• Some users who have previously installed versions of the RcppEigen and minqa packages may encounter segmentation faults (!!); the solution is to make sure to re-install these packages before installing **lme4**. (Because the problem is not with the explicit *version* of the packages, but with running packages that were built with different versions of **Rcpp** in conjunction with each other, simply making sure you have the latest version, or using update.packages, will not necessarily solve the problem; you must actually re-install the packages. The problem is most likely with **minqa**.)

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Arabidopsis

Arabidopsis clipping/fertilization data

#### **Description**

Data on genetic variation in responses to fertilization and simulated herbivory in Arabidopsis

# Usage

```
data("Arabidopsis")
```

#### **Format**

A data frame with 625 observations on the following 8 variables.

```
reg region: a factor with 3 levels NL (Netherlands), SP (Spain), SW (Sweden)
popul population: a factor with the form n.R representing a population in region R
gen genotype: a factor with 24 (numeric-valued) levels
rack a nuisance factor with 2 levels, one for each of two greenhouse racks
nutrient fertilization treatment/nutrient level (1, minimal nutrients or 8, added nutrients)
amd simulated herbivory or "clipping" (apical meristem damage): unclipped (baseline) or clipped
status a nuisance factor for germination method (Normal, Petri.Plate, or Transplant)
total.fruits total fruit set per plant (integer)
```

#### Source

From Josh Banta

## References

Joshua A. Banta, Martin H. H Stevens, and Massimo Pigliucci (2010) A comprehensive test of the 'limiting resources' framework applied to plant tolerance to apical meristem damage. *Oikos* **119**(2), 359–369; http://dx.doi.org/10.1111/j.1600-0706.2009.17726.x

6 bootMer

bootMer

Model-based (Semi-)Parametric Bootstrap for Mixed Models

# Description

Perform model-based (Semi-)parametric bootstrap for mixed models.

# Usage

```
bootMer(x, FUN, nsim = 1, seed = NULL, use.u = FALSE, re.form=NA,
type = c("parametric", "semiparametric"),
verbose = FALSE, .progress = "none", PBargs = list(),
parallel = c("no", "multicore", "snow"),
ncpus = getOption("boot.ncpus", 1L), cl = NULL)
```

# **Arguments**

Χ	a fitted merMod object: see lmer, glmer, etc.
FUN	a function taking a fitted merMod object as input and returning the <i>statistic</i> of interest, which must be a (possibly named) numeric vector.
nsim	number of simulations, positive integer; the bootstrap $B$ (or $R$ ).
seed	optional argument to set.seed.
use.u	logical, indicating whether the spherical random effects should be simulated / bootstrapped as well. If TRUE, they are not changed, and all inference is conditional on these values. If FALSE, new normal deviates are drawn (see Details).
re.form	formula, NA (equivalent to use.u=FALSE), or NULL (equivalent to use.u=TRUE): alternative to use.u for specifying which random effects to incorporate. See simulate.merMod for details.
type	character string specifying the type of bootstrap, "parametric" or "semiparametric"; partial matching is allowed.
verbose	logical indicating if progress should print output
.progress	character string - type of progress bar to display. Default is "none"; the function will look for a relevant *ProgressBar function, so "txt" will work in general; "tk" is available if the <b>tcltk</b> package is loaded; or "win" on Windows systems. Progress bars are disabled (with a message) for parallel operation.
PBargs	a list of additional arguments to the progress bar function (the package authors like list(style=3)).
parallel	The type of parallel operation to be used (if any). If missing, the default is taken from the option "boot.parallel" (and if that is not set, "no").
ncpus	integer: number of processes to be used in parallel operation: typically one would choose this to be the number of available CPUs.
cl	An optional <b>parallel</b> or <b>snow</b> cluster for use if parallel = "snow". If not supplied, a cluster on the local machine is created for the duration of the boot call.

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#### **Details**

The semi-parametric variant is only partially implemented, and we only provide a method for lmer and glmer results.

The working name for bootMer() was "simulestimate()", as it is an extension of simulate (see simulate.merMod), but we want to emphasize its potential for valid inference.

- If use.u is FALSE and type is "parametric", each simulation generates new values of both the "spherical" random effects u and the i.i.d. errors ε, using rnorm() with parameters corresponding to the fitted model x.
- If use.u is TRUE and type=="parametric", only the i.i.d. errors (or, for GLMMs, response values drawn from the appropriate distributions) are resampled, with the values of u staying fixed at their estimated values.
- If use.u is TRUE and type=="semiparametric", the i.i.d. errors are sampled from the distribution of (response) residuals. (For GLMMs, the resulting sample will no longer have the same properties as the original sample, and the method may not make sense; a warning is generated.) The semiparametric bootstrap is currently an experimental feature, and therefore may not be stable.
- The case where use.u is FALSE and type=="semiparametric" is not implemented; Morris (2002) suggests that resampling from the estimated values of u is not good practice.

#### Value

an object of S3 class "boot", compatible with boot package's boot() result.

#### Note

If you are using parallel="snow", you will need to run clusterEvalQ(cl,library("lme4")) before calling bootMer to make sure that the lme4 package is loaded on all of the workers; you may additionally need to use clusterExport if you are using a summary function that calls any objects from the environment.

#### References

Davison, A.C. and Hinkley, D.V. (1997) *Bootstrap Methods and Their Application*. Cambridge University Press.

Morris, J. S. (2002). The BLUPs Are Not 'best' When It Comes to Bootstrapping. *Statistics & Probability Letters* **56**(4): 425–430. doi:10.1016/S0167-7152(02)00041-X.

# See Also

- confint.merMod, for a more specific approach to bootstrap confidence intervals on parameters.
- refit(), or PBmodcomp() from the pbkrtest package, for parametric bootstrap comparison of models.
- boot(), and then boot.ci, from the boot package.
- profile-methods, for likelihood-based inference, including confidence intervals.
- pvalues, for more general approaches to inference and p-value computation in mixed models.

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```
fm01ML <- lmer(Yield ~ 1|Batch, Dyestuff, REML = FALSE)</pre>
## see ?"profile-methods"
mySumm <- function(.) { s <- sigma(.)</pre>
    c(beta =getME(., "beta"), sigma = s, sig01 = unname(s * getME(., "theta"))) }
(t0 <- mySumm(fm01ML)) # just three parameters</pre>
## alternatively:
mySumm2 <- function(.) {</pre>
   c(beta=fixef(.), sigma=sigma(.), sig01=sqrt(unlist(VarCorr(.))))
}
set.seed(101)
## 3.8s (on a 5600 MIPS 64bit fast(year 2009) desktop "AMD Phenom(tm) II X4 925"):
system.time( boo01 <- bootMer(fm01ML, mySumm, nsim = 100) )</pre>
## to "look" at it
if (requireNamespace("boot")) {
   boo@1
    ## note large estimated bias for sig01
    ## (~30% low, decreases _slightly_ for nsim = 1000)
    ## extract the bootstrapped values as a data frame ...
    head(as.data.frame(boo01))
    ## ----- Bootstrap-based confidence intervals ------
    ## warnings about "Some ... intervals may be unstable" go away
    ## for larger bootstrap samples, e.g. nsim=500
    ## intercept
    (bCI.1 <- boot::boot.ci(boo01, index=1, type=c("norm", "basic", "perc")))# beta
    ## Residual standard deviation - original scale:
    (bCI.2 <- boot::boot.ci(boo01, index=2, type=c("norm", "basic", "perc")))
    ## Residual SD - transform to log scale:
    (bCI.2L <- boot::boot.ci(boo01, index=2, type=c("norm", "basic", "perc"),
                       h = log, hdot = function(.) 1/., hinv = exp))
    ## Among-batch variance:
    (bCI.3 <- boot::boot.ci(boo01, index=3, type=c("norm", "basic", "perc"))) # sig01
    ## Copy of unexported stats:::format.perc helper function
    format.perc <- function(probs, digits) {</pre>
        paste(format(100 * probs, trim = TRUE,
                     scientific = FALSE, digits = digits),
              "%")
    }
    ## Extract all CIs (somewhat awkward)
   bCI.tab <- function(b,ind=length(b$t0), type="perc", conf=0.95) {
       btab0 <- t(sapply(as.list(seq(ind)),</pre>
```

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```
function(i)
            boot::boot.ci(b,index=i,conf=conf, type=type)$percent))
        btab <- btab0[,4:5]</pre>
        rownames(btab) <- names(b$t0)</pre>
        a <- (1 - conf)/2
        a <- c(a, 1 - a)
        pct <- format.perc(a, 3)</pre>
        colnames(btab) <- pct</pre>
        return(btab)
   bCI.tab(boo01)
    ## Graphical examination:
   plot(boo01,index=3)
    ## Check stored values from a longer (1000-replicate) run:
    (load(system.file("testdata","boo01L.RData", package="lme4")))# "boo01L"
   plot(boo01L, index=3)
   mean(boo01L$t[,"sig01"]==0) ## note point mass at zero!
} ## if boot package available
```

cake

Breakage Angle of Chocolate Cakes

## **Description**

Data on the breakage angle of chocolate cakes made with three different recipes and baked at six different temperatures. This is a split-plot design with the recipes being whole-units and the different temperatures being applied to sub-units (within replicates). The experimental notes suggest that the replicate numbering represents temporal ordering.

## Format

A data frame with 270 observations on the following 5 variables.

```
replicate a factor with levels 1 to 15 recipe a factor with levels A, B and C temperature an ordered factor with levels 175 < 185 < 195 < 205 < 215 < 225 angle a numeric vector giving the angle at which the cake broke. temp numeric value of the baking temperature (degrees F).
```

## Details

The replicate factor is nested within the recipe factor, and temperature is nested within replicate.

## Source

Original data were presented in Cook (1938), and reported in Cochran and Cox (1957, p. 300). Also cited in Lee, Nelder and Pawitan (2006).

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#### References

Cook, F. E. (1938) *Chocolate cake, I. Optimum baking temperature*. Master's Thesis, Iowa State College.

Cochran, W. G., and Cox, G. M. (1957) *Experimental designs*, 2nd Ed. New York, John Wiley & Sons.

Lee, Y., Nelder, J. A., and Pawitan, Y. (2006) *Generalized linear models with random effects. Unified analysis via H-likelihood.* Boca Raton, Chapman and Hall/CRC.

# **Examples**

cbpp

Contagious bovine pleuropneumonia

## **Description**

Contagious bovine pleuropneumonia (CBPP) is a major disease of cattle in Africa, caused by a mycoplasma. This dataset describes the serological incidence of CBPP in zebu cattle during a follow-up survey implemented in 15 commercial herds located in the Boji district of Ethiopia. The goal of the survey was to study the within-herd spread of CBPP in newly infected herds. Blood samples were quarterly collected from all animals of these herds to determine their CBPP status. These data were used to compute the serological incidence of CBPP (new cases occurring during a given time period). Some data are missing (lost to follow-up).

#### **Format**

A data frame with 56 observations on the following 4 variables.

```
herd A factor identifying the herd (1 to 15).
```

incidence The number of new serological cases for a given herd and time period.

size A numeric vector describing herd size at the beginning of a given time period.

period A factor with levels 1 to 4.

#### **Details**

Serological status was determined using a competitive enzyme-linked immuno-sorbent assay (cELISA).

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## Source

Lesnoff, M., Laval, G., Bonnet, P., Abdicho, S., Workalemahu, A., Kifle, D., Peyraud, A., Lancelot, R., Thiaucourt, F. (2004) Within-herd spread of contagious bovine pleuropneumonia in Ethiopian highlands. *Preventive Veterinary Medicine* **64**, 27–40.

# **Examples**

checkConv

Extended Convergence Checking

# **Description**

Primarily internal code for checking optimization convergence, see convergence for a more detailed discussion.

# Usage

```
checkConv(derivs, coefs, ctrl, lbound, debug = FALSE)
```

# Arguments

derivs	typically the "derivs" attribute of optimizeLmer(); with "gradients" and possibly "Hessian" component
coefs	current coefficient estimates
ctrl	list of lists, each with action character strings specifying what should happen when a check triggers, and tol numerical tolerances, as is the result of <a href="mailto:lmerControl">lmerControl</a> ()\$checkConv.
1bound	vector of lower bounds for random-effects parameters only (length is taken to determine number of RE parameters)
debug	enable debugging output, useful if some checks are on "ignore", but would "trigger"

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#### Value

A result list containing

code The return code for the check

messages A character vector of warnings and messages generated by the check

## See Also

convergence

confint.merMod

Compute Confidence Intervals for Parameters of a [ng]lmer Fit

## **Description**

Compute confidence intervals on the parameters of a \*lmer() model fit (of class"merMod").

# Usage

# **Arguments**

object a fitted [ng]lmer model or profile

parm parameters for which intervals are sought. Specified by an integer vector of

positions, character vector of parameter names, or (unless doing parametric bootstrapping with a user-specified bootstrap function) "theta\_" or "beta\_" to specify variance-covariance or fixed effects parameters only: see the which

parameter of profile.

level confidence level < 1, typically above 0.90.

method a character string determining the method for computing the confidence inter-

vals.

zeta (for method = "profile" only:) likelihood cutoff (if not specified, as by de-

fault, computed from level).

nsim number of simulations for parametric bootstrap intervals.

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FUN	bootstrap function; if NULL, an internal function that returns the fixed-effect parameters as well as the random-effect parameters on the standard deviation/correlation scale will be used. See bootMer for details.
boot.type	bootstrap confidence interval type, as described in boot.ci. (Methods 'stud' and 'bca' are unavailable because they require additional components to be calculated.)
quiet	(logical) suppress messages about computationally intensive profiling?
oldNames	(logical) use old-style names for variance-covariance parameters, e.g. ".sig01", rather than newer (more informative) names such as "sd_(Intercept) Subject"? (See signames argument to profile).
non.mono.tol	tolerance for detecting a non-monotonic profile and warning/falling back to linear interpolation
•••	additional parameters to be passed to profile.merMod or bootMer, respectively.

#### **Details**

Depending on the method specified, confint() computes confidence intervals by

"profile": computing a likelihood profile and finding the appropriate cutoffs based on the likelihood ratio test;

"Wald": approximating the confidence intervals (of fixed-effect parameters only; all variance-covariance parameters CIs will be returned as NA) based on the estimated local curvature of the likelihood surface;

"boot": performing parametric bootstrapping with confidence intervals computed from the bootstrap distribution according to boot.type (see bootMer, boot.ci).

## Value

a numeric table (matrix with column and row names) of confidence intervals; the confidence intervals are computed on the standard deviation scale.

# Note

The default method "profile" amounts to

where the profile method profile.merMod does almost all the computations. Therefore it is typically advisable to store the profile(.) result, say in pp, and then use confint(pp, level=\*) e.g., for different levels.

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## **Examples**

convergence

Assessing Convergence for Fitted Models

## **Description**

The **lme4** package uses general-purpose nonlinear optimizers (e.g. Nelder-Mead or Powell's BOBYQA method) to estimate the variance-covariance matrices of the random effects. Assessing reliably whether such algorithms have converged is difficult. For example, evaluating the Karush-Kuhn-Tucker conditions (convergence criteria which in the simplest case of non-constrained optimization reduce to showing that the gradient is zero and the Hessian is positive definite) is challenging because of the difficulty of evaluating the gradient and Hessian.

We (the 1me4 authors and maintainers) are still in the process of finding the best strategies for testing convergence. Some of the relevant issues are

- the gradient and Hessian are the basic ingredients of KKT-style testing, but when they have
  to be estimated by finite differences (as in the case of lme4; direct computation of derivatives
  based on analytic expressions may eventually be available for some special classes, but we
  have not yet implemented them) they may not be sufficiently accurate for reliable convergence
  testing.
- The Hessian computation in particular represents a difficult tradeoff between computational expense and accuracy. At present the Hessian computations used for convergence checking (and for estimating standard errors of fixed-effect parameters for GLMMs) follow the **ordinal** package in using a naive but computationally cheap centered finite difference computation (with a fixed step size of 10<sup>-4</sup>). A more reliable but more expensive approach is to use Richardson extrapolation, as implemented in the **numDeriv** package.
- it is important to scale the estimated gradient at the estimate appropriately; two reasonable approaches are

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 don't scale random-effects (Cholesky) gradients, since these are essentially already unitless (for LMMs they are scaled relative to the residual variance; for GLMMs they are scaled relative to the sampling variance of the conditional distribution); for GLMMs, scale fixed-effect gradients by the standard deviations of the corresponding input variable, or

- 2. scale gradients by the inverse Cholesky factor of the Hessian, equivalent to scaling by the estimated Wald standard error of the estimated parameters. The latter approach is used in the current version of **lme4**; it has the disadvantage that it requires us to estimate the Hessian (although the Hessian is required for reliable estimation of the fixed-effect standard errors for GLMMs in any case).
- Exploratory analyses suggest that (1) the naive estimation of the Hessian may fail for large data sets (number of observations greater than approximately  $10^5$ ); (2) the magnitude of the scaled gradient increases with sample size, so that warnings will occur even for apparently well-behaved fits with large data sets.

If you do see convergence warnings, and want to trouble-shoot/double-check the results, the following steps are recommended (examples are given below):

- · double-check the model specification and the data for mistakes
- center and scale continuous predictor variables (e.g. with scale)
- check for singularity: if any of the diagonal elements of the Cholesky factor are zero or very small, the convergence testing methods may be inappropriate (see examples)
- double-check the Hessian calculation with the more expensive Richardson extrapolation method (see examples)
- restart the fit from the apparent optimum, or from a point perturbed slightly away from the optimum
- try all available optimizers (e.g. several different implementations of BOBYQA and Nelder-Mead, L-BFGS-B from optim, nlminb, ...) via the allFit() function, see '5.' in the examples. While this will of course be slow for large fits, we consider it the gold standard; if all optimizers converge to values that are practically equivalent, then we would consider the convergence warnings to be false positives.

To quote Douglas Adams, we apologize for the inconvenience.

#### See Also

lmerControl

```
fm1 <- lmer(Reaction ~ Days + (Days | Subject), sleepstudy)
## 1. center and scale predictors:
ss.CS <- transform(sleepstudy, Days=scale(Days))
fm1.CS <- update(fm1, data=ss.CS)

## 2. check singularity
diag.vals <- getME(fm1,"theta")[getME(fm1,"lower") == 0]
any(diag.vals < 1e-6) # FALSE</pre>
```

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```
## 3. recompute gradient and Hessian with Richardson extrapolation
devfun <- update(fm1, devFunOnly=TRUE)</pre>
if (isLMM(fm1)) {
    pars <- getME(fm1,"theta")</pre>
} else {
    ## GLMM: requires both random and fixed parameters
   pars <- getME(fm1, c("theta", "fixef"))</pre>
if (require("numDeriv")) {
   cat("hess:\n"); print(hess <- hessian(devfun, unlist(pars)))</pre>
   cat("grad:\n"); print(grad <- grad(devfun, unlist(pars)))</pre>
    cat("scaled gradient:\n")
    print(scgrad <- solve(chol(hess), grad))</pre>
}
## compare with internal calculations:
fm1@optinfo$derivs
## 4. restart the fit from the original value (or
## a slightly perturbed value):
fm1.restart <- update(fm1, start=pars)</pre>
## 5. try all available optimizers
 source(system.file("utils", "allFit.R", package="lme4"))
 fm1.all <- allFit(fm1)</pre>
 ss <- summary(fm1.all)</pre>
 ss$ fixef
                           ## extract fixed effects
 ss$ llik
                           ## log-likelihoods
 ss$ sdcor
                          ## SDs and correlations
 ss$ theta
                          ## Cholesky factors
 ss$ which.OK
                          ## which fits worked
```

devcomp

Extract the deviance component list

# Description

Return the deviance component list

# Usage

```
devcomp(x)
```

## **Arguments**

Х

a fitted model of class merMod

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#### **Details**

A fitted model of class merMod has a devcomp slot as described in the value section.

#### Value

a list with components

dims a named integer vector of various dimensions

cmp a named numeric vector of components of the deviance

#### Note

This function is deprecated, use getME(., "devcomp")

drop1.merMod

Drop all possible single fixed-effect terms from a mixed effect model

## **Description**

Drop allowable single terms from the model: see drop1 for details of how the appropriate scope for dropping terms is determined.

# Usage

```
## S3 method for class 'merMod'
drop1(object, scope, scale = 0,
    test = c("none", "Chisq", "user"),
    k = 2, trace = FALSE, sumFun, ...)
```

## **Arguments**

object	a fitted merMod object.	

scope a formula giving the terms to be considered for adding or dropping.

scale Currently ignored (included for S3 method compatibility)

test should the results include a test statistic relative to the original model? The  $\chi^2$ 

test is a likelihood-ratio test, which is approximate due to finite-size effects.

k the penalty constant in AIC trace print tracing information?

sumFun a summary function to be used when test=="user". It must allow arguments

scale and k, but these may be ignored (e.g. specified in dots). The first two arguments must be object, the full model fit, and objectDrop, a reduced model. If objectDrop is missing, sumFun should return a vector of with the appropriate

length and names (the actual contents are ignored).

... other arguments (ignored)

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#### **Details**

drop1 relies on being able to find the appropriate information within the environment of the formula of the original model. If the formula is created in an environment that does not contain the data, or other variables passed to the original model (for example, if a separate function is called to define the formula), then drop1 will fail. A workaround (see example below) is to manually specify an appropriate environment for the formula.

## Value

An object of class anova summarizing the differences in fit between the models.

```
fm1 <- lmer(Reaction~Days+(Days|Subject),sleepstudy)</pre>
## likelihood ratio tests
drop1(fm1,test="Chisq")
## use Kenward-Roger corrected F test, or parametric bootstrap,
## to test the significance of each dropped predictor
if (require(pbkrtest) && packageVersion("pbkrtest")>="0.3.8") {
   KRSumFun <- function(object, objectDrop, ...) {</pre>
      krnames <- c("ndf","ddf","Fstat","p.value","F.scaling")</pre>
      r <- if (missing(objectDrop)) {</pre>
          setNames(rep(NA,length(krnames)),krnames)
         krtest <- KRmodcomp(object,objectDrop)</pre>
         unlist(krtest$stats[krnames])
      attr(r, "method") <- c("Kenward-Roger via pbkrtest package")</pre>
   drop1(fm1,test="user",sumFun=KRSumFun)
   if(lme4:::testLevel() >= 3) { ## takes about 16 sec
     nsim <- 100
     PBSumFun <- function(object, objectDrop, ...) {</pre>
pbnames <- c("stat","p.value")</pre>
r <- if (missing(objectDrop)) {</pre>
    setNames(rep(NA,length(pbnames)),pbnames)
} else {
   pbtest <- PBmodcomp(object,objectDrop,nsim=nsim)</pre>
   unlist(pbtest$test[2,pbnames])
}
attr(r, "method") <- c("Parametric bootstrap via pbkrtest package")</pre>
     system.time(drop1(fm1,test="user",sumFun=PBSumFun))
}
## workaround for creating a formula in a separate environment
createFormula <- function(resp, fixed, rand) {</pre>
    f <- reformulate(c(fixed,rand),response=resp)</pre>
    ## use the parent (createModel) environment, not the
```

dummy 19

```
## environment of this function (which does not contain 'data')
    environment(f) <- parent.frame()
    f
}
createModel <- function(data) {
    mf.final <- createFormula("Reaction", "Days", "(Days|Subject)")
    lmer(mf.final, data=data)
}
drop1(createModel(data=sleepstudy))</pre>
```

dummy

Dummy variables (experimental)

## **Description**

Largely a wrapper for model.matrix that accepts a factor, f, and returns a dummy matrix with nlevels(f)-1 columns (the first column is dropped by default). Useful whenever one wishes to avoid the behaviour of model.matrix of always returning an nlevels(f)-column matrix, either by the addition of an intercept column, or by keeping one column for all levels.

# Usage

```
dummy(f, levelsToKeep)
```

# **Arguments**

f An object coercible to factor.

levelsToKeep An optional character vector giving the subset of levels(f) to be converted to dummy variables.

## Value

A model.matrix with dummy variables as columns.

20 Dyestuff

Dyestuff

Yield of dyestuff by batch

#### **Description**

The Dyestuff data frame provides the yield of dyestuff (Naphthalene Black 12B) from 5 different preparations from each of 6 different batchs of an intermediate product (H-acid). The Dyestuff2 data were generated data in the same structure but with a large residual variance relative to the batch variance.

#### **Format**

Data frames, each with 30 observations on the following 2 variables.

Batch a factor indicating the batch of the intermediate product from which the preparation was created.

Yield the yield of dyestuff from the preparation (grams of standard color).

#### **Details**

The Dyestuff data are described in Davies and Goldsmith (1972) as coming from "an investigation to find out how much the variation from batch to batch in the quality of an intermediate product (H-acid) contributes to the variation in the yield of the dyestuff (Naphthalene Black 12B) made from it. In the experiment six samples of the intermediate, representing different batches of works manufacture, were obtained, and five preparations of the dyestuff were made in the laboratory from each sample. The equivalent yield of each preparation as grams of standard colour was determined by dye-trial."

The Dyestuff2 data are described in Box and Tiao (1973) as illustrating "the case where between-batches mean square is less than the within-batches mean square. These data had to be constructed for although examples of this sort undoubtably occur in practice, they seem to be rarely published."

#### **Source**

O.L. Davies and P.L. Goldsmith (eds), *Statistical Methods in Research and Production*, 4th ed., Oliver and Boyd, (1972), section 6.4

G.E.P. Box and G.C. Tiao, *Bayesian Inference in Statistical Analysis*, Addison-Wesley, (1973), section 5.1.2

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expandDoubleVerts

Expand terms with '||' notation into separate '|' terms

# Description

From the right hand side of a formula for a mixed-effects model, expand terms with the double vertical bar operator into separate, independent random effect terms.

# Usage

```
expandDoubleVerts(term)
```

## **Arguments**

term

a mixed-model formula

#### Value

the modified term

## Note

Because | | works at the level of formula parsing, it has no way of knowing whether a variable is a factor. It just takes the terms within a random-effects term and literally splits them into the intercept and separate no-intercept terms, e.g. (1+x+y|f) would be split into (1|f) + (0+x|f) + (0+y|f). However, | | will fail to break up factors into separate terms; the dummy function can be useful in this case, although it is not as convenient as | |.

## See Also

```
formula, model.frame, model.matrix, dummy.
Other utilities: mkRespMod, mkReTrms, nlformula, nobars, subbars
```

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factorize

Attempt to convert grouping variables to factors

# **Description**

If variables within a data frame are not factors, try to convert them. Not intended for end-user use; this is a utility function that needs to be exported, for technical reasons.

# Usage

```
factorize(x,frloc,char.only=FALSE)
```

## **Arguments**

x a formula frloc a data frame

char.only (logical) convert only character variables to factors?

## Value

a copy of the data frame with factors converted

findbars

Determine random-effects expressions from a formula

# **Description**

From the right hand side of a formula for a mixed-effects model, determine the pairs of expressions that are separated by the vertical bar operator. Also expand the slash operator in grouping factor expressions and expand terms with the double vertical bar operator into separate, independent random effect terms.

## Usage

```
findbars(term)
```

## **Arguments**

term

a mixed-model formula

fixef 23

#### Value

pairs of expressions that were separated by vertical bars

#### Note

This function is called recursively on individual terms in the model, which is why the argument is called term and not a name like form, indicating a formula.

#### See Also

```
formula, model.frame, model.matrix.

Other utilities: mkRespMod, mkReTrms, nlformula, nobars, subbars
```

## **Examples**

```
findbars(f1 <- Reaction ~ Days + (Days | Subject))
## => list( Days | Subject )
## These two are equivalent:% tests in ../inst/tests/test-doubleVertNotation.R
findbars(y ~ Days + (1 | Subject) + (0 + Days | Subject))
findbars(y ~ Days + (Days || Subject))
## => list of length 2: list (1 | Subject , 0 + Days | Subject)
findbars(~ 1 + (1 | batch / cask))
## => list of length 2: list (1 | cask:batch , 1 | batch)
```

fixef

Extract fixed-effects estimates

#### **Description**

Extract the fixed-effects estimates

## Usage

```
## S3 method for class 'merMod'
fixef(object, add.dropped=FALSE, ...)
```

## **Arguments**

```
object any fitted model object from which fixed effects estimates can be extracted.

add.dropped for models with rank-deficient design matrix, reconstitute the full-length parameter vector by adding NA values in appropriate locations?

optional additional arguments. Currently none are used in any methods.
```

## **Details**

Extract the estimates of the fixed-effects parameters from a fitted model.

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## Value

a named, numeric vector of fixed-effects estimates.

## **Examples**

fortify

add information to data based on a fitted model

# **Description**

add information to data based on a fitted model

# Usage

```
fortify.merMod(model, data = getData(model),
    ...)
```

# Arguments

```
model fitted model
data original data set, if needed
... additional arguments
```

# **Details**

fortify is a function defined in the **ggplot2** package, q.v. for more details. fortify is *not* defined here, and fortify.merMod is defined as a function rather than an S3 method, to avoid (1) inducing a dependency on **ggplot2** or (2) masking methods from **ggplot2**. This is currently an experimental feature.

getME 25

getME

Extract or Get Generalized Components from a Fitted Mixed Effects Model

# **Description**

Extract (or "get") "components" – in a generalized sense – from a fitted mixed-effects model, i.e., (in this version of the package) from an object of class "merMod".

# Usage

# **Arguments**

object

a fitted mixed-effects model of class "merMod", i.e., typically the result of lmer(), glmer() or nlmer().

name

a character vector specifying the name(s) of the "component". If length(name) > 1 or if name = "ALL", a named list of components will be returned. Possible values are:

"X": fixed-effects model matrix

"Z": random-effects model matrix

"Zt": transpose of random-effects model matrix. Note that the structure of Zt has changed since lme4.0; to get a backward-compatible structure, use do.call(Matrix::rBind,getME(.,"Ztlist"))

"Ztlist": list of components of the transpose of the random-effects model matrix, separated by individual variance component

"mmList": list of raw model matrices associated with random effects terms

"y": response vector

"mu": conditional mean of the response

"u": conditional mode of the "spherical" random effects variable

"b": conditional mode of the random effects variable

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"Gp": groups pointer vector. A pointer to the beginning of each group of random effects corresponding to the random-effects terms, beginning with 0 and including a final element giving the total number of random effects

"Tp": theta pointer vector. A pointer to the beginning of the theta sub-vectors corresponding to the random-effects terms, beginning with 0 and including a final element giving the number of thetas.

"L": sparse Cholesky factor of the penalized random-effects model.

"Lambda": relative covariance factor  $\Lambda$  of the random effects.

"Lambdat": transpose  $\Lambda'$  of  $\Lambda$  above.

"Lind": index vector for inserting elements of  $\theta$  into the nonzeros of  $\Lambda$ .

"Tlist": vector of template matrices from which the blocks of  $\Lambda$  are generated.

"A": Scaled sparse model matrix (class "dgCMatrix") for the unit, orthogonal random effects, U, equal to getME(.,"Zt") %\*% getME(.,"Lambdat")

"RX": Cholesky factor for the fixed-effects parameters

"RZX": cross-term in the full Cholesky factor

"sigma": residual standard error; note that sigma(object) is preferred.

"flist": a list of the grouping variables (factors) involved in the random effect terms

"fixef": fixed-effects parameter estimates

"beta": fixed-effects parameter estimates (identical to the result of fixef, but without names)

"theta": random-effects parameter estimates: these are parameterized as the relative Cholesky factors of each random effect term

"ST": A list of S and T factors in the TSST' Cholesky factorization of the relative variance matrices of the random effects associated with each random-effects term. The unit lower triangular matrix, T, and the diagonal matrix, S, for each term are stored as a single matrix with diagonal elements from S and off-diagonal elements from T.

"n\_rtrms": number of random-effects terms

"n\_rfacs": number of distinct random-effects grouping factors

"N": number of rows of X

"n": length of the response vector, y

"p": number of columns of the fixed effects model matrix, X

"q": number of columns of the random effects model matrix, Z

"p\_i": numbers of columns of the raw model matrices, mmList

"1\_i": numbers of levels of the grouping factors

"q\_i": numbers of columns of the term-wise model matrices, ZtList

"k": number of random effects terms

"m\_i": numbers of covariance parameters in each term

"m": total number of covariance parameters

"cnms": the "component names", a list.

"REML": 0 indicates the model was fitted by maximum likelihood, any other positive integer indicates fitting by restricted maximum likelihood

"is\_REML": same as the result of isREML(.)

"devcomp": a list consisting of a named numeric vector, cmp, and a named integer vector, dims, describing the fitted model. The elements of cmp are:

ldL2 twice the log determinant of L

IdRX2 twice the log determinant of RX

wrss weighted residual sum of squares

ussq squared length of u

pwrss penalized weighted residual sum of squares, "wrss + ussq"

drsum sum of residual deviance (GLMMs only)

**REML** REML criterion at optimum (LMMs fit by REML only)

**dev** deviance criterion at optimum (models fit by ML only)

sigmaML ML estimate of residual standard deviation

sigmaREML REML estimate of residual standard deviation

**tolPwrss** tolerance for declaring convergence in the penalized iteratively weighted residual sum-of-squares (GLMMs only)

The elements of dims are:

N number of rows of X

**n** length of y

**p** number of columns of X

nmp n-p

**nth** length of theta

q number of columns of Z

nAGQ see glmer

compDev see glmerControl

useSc TRUE if model has a scale parameter

reTrms number of random effects terms

**REML** 0 indicates the model was fitted by maximum likelihood, any other positive integer indicates fitting by restricted maximum likelihood

**GLMM** TRUE if a GLMM

**NLMM** TRUE if an NLMM

"offset": model offset

"lower": lower bounds on model parameters (random effects parameters only).

"devfun": deviance function (so far only available for LMMs)

"glmer.nb. theta": negative binomial  $\theta$  parameter, only for glmer.nb.

"ALL": get all of the above as a list.

currently unused in lme4, potentially further arguments in methods.

# Details

The goal is to provide "everything a user may want" from a fitted "merMod" object as far as it is not available by methods, such as fixef, ranef, vcov, etc.

28 GHrule

## Value

Unspecified, as very much depending on the name.

## See Also

```
getCall(). More standard methods for "merMod" objects, such as ranef, fixef, vcov, etc.: see
methods(class="merMod")
```

## **Examples**

GHrule

Univariate Gauss-Hermite quadrature rule

## **Description**

Create a univariate Gauss-Hermite quadrature rule.

## Usage

```
GHrule(ord, asMatrix = TRUE)
```

## **Arguments**

ord

scalar integer between 1 and 25 - the order, or number of nodes and weights, in the rule. When the function being multiplied by the standard normal density is

a polynomial of order 2k-1 the rule of order k integrates the product exactly.

asMatrix

logical scalar - should the result be returned as a matrix. If FALSE a data frame

is returned. Defaults to TRUE.

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#### **Details**

This version of Gauss-Hermite quadrature provides the node positions and weights for a scalar integral of a function multiplied by the standard normal density.

Originally based on package **SparseGrid**'s hidden GQN().

#### Value

a matrix (or data frame, is asMatrix is false) with ord rows and three columns which are z the node positions, w the weights and ldnorm, the logarithm of the normal density evaluated at the nodes.

#### See Also

a different interface is available via GQdk().

#### **Examples**

```
(r5 <- GHrule(5, asMatrix=FALSE))
## second, fourth, sixth, eighth and tenth central moments of the
## standard Gaussian density
with(r5, sapply(seq(2, 10, 2), function(p) sum(w * z^p)))</pre>
```

glmer

Fitting Generalized Linear Mixed-Effects Models

## Description

Fit a generalized linear mixed-effects model (GLMM). Both fixed effects and random effects are specified via the model formula.

## Usage

```
glmer(formula, data = NULL, family = gaussian, control = glmerControl(),
    start = NULL, verbose = 0L, nAGQ = 1L, subset, weights, na.action,
    offset, contrasts = NULL, mustart, etastart,
    devFunOnly = FALSE, ...)
```

## **Arguments**

formula

a two-sided linear formula object describing both the fixed-effects and random-effects part of the model, with the response on the left of a ~ operator and the terms, separated by + operators, on the right. Random-effects terms are distinguished by vertical bars ("|") separating expressions for design matrices from grouping factors.

30 glmer

data

an optional data frame containing the variables named in formula. By default the variables are taken from the environment from which 1mer is called. While data is optional, the package authors strongly recommend its use, especially when later applying methods such as update and drop1 to the fitted model (such methods are not guaranteed to work properly if data is omitted). If data is omitted, variables will be taken from the environment of formula (if specified as a formula) or from the parent frame (if specified as a character vector).

family

a GLM family, see glm and family.

control

a list (of correct class, resulting from lmerControl() or glmerControl() respectively) containing control parameters, including the nonlinear optimizer to be used and parameters to be passed through to the nonlinear optimizer, see the \*lmerControl documentation for details.

start

a named list of starting values for the parameters in the model, or a numeric vector. A numeric start argument will be used as the starting value of theta. If start is a list, the theta element (a numeric vector) is used as the starting value for the first optimization step (default=1 for diagonal elements and 0 for off-diagonal elements of the lower Cholesky factor); the fitted value of theta from the first step, plus start[["fixef"]], are used as starting values for the second optimization step. If start has both fixef and theta elements, the first optimization step is skipped. For more details or finer control of optimization, see modular.

verbose

integer scalar. If > 0 verbose output is generated during the optimization of the parameter estimates. If > 1 verbose output is generated during the individual PIRLS steps.

nAGQ

integer scalar - the number of points per axis for evaluating the adaptive Gauss-Hermite approximation to the log-likelihood. Defaults to 1, corresponding to the Laplace approximation. Values greater than 1 produce greater accuracy in the evaluation of the log-likelihood at the expense of speed. A value of zero uses a faster but less exact form of parameter estimation for GLMMs by optimizing the random effects and the fixed-effects coefficients in the penalized iteratively reweighted least squares step. (See Details.)

subset

an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.

weights

an optional vector of 'prior weights' to be used in the fitting process. Should be NULL or a numeric vector.

na.action

a function that indicates what should happen when the data contain NAs. The default action (na.omit, inherited from the 'factory fresh' value of getOption("na.action")) strips any observations with any missing values in any variables.

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.

contrasts

an optional list. See the contrasts.arg of model.matrix.default.

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mustart	optional starting values on the scale of the conditional mean, as in glm; see there for details.
etastart	optional starting values on the scale of the unbounded predictor as in glm; see there for details.
devFunOnly	logical - return only the deviance evaluation function. Note that because the deviance function operates on variables stored in its environment, it may not return <i>exactly</i> the same values on subsequent calls (but the results should always be within machine tolerance).
	other potential arguments. A method argument was used in earlier versions of the package. Its functionality has been replaced by the nAGO argument.

#### **Details**

Fit a generalized linear mixed model, which incorporates both fixed-effects parameters and random effects in a linear predictor, via maximum likelihood. The linear predictor is related to the conditional mean of the response through the inverse link function defined in the GLM family.

The expression for the likelihood of a mixed-effects model is an integral over the random effects space. For a linear mixed-effects model (LMM), as fit by lmer, this integral can be evaluated exactly. For a GLMM the integral must be approximated. The most reliable approximation for GLMMs is adaptive Gauss-Hermite quadrature, at present implemented only for models with a single scalar random effect. The nAGQ argument controls the number of nodes in the quadrature formula. A model with a single, scalar random-effects term could reasonably use up to 25 quadrature points per scalar integral.

# Value

An object of class merMod (more specifically, an object of *subclass* glmerMod) for which many methods are available (e.g. methods(class="merMod"))

#### See Also

lmer (for details on formulas and parameterization); glm for Generalized Linear Models (without random effects). nlmer for nonlinear mixed-effects models.

glmer.nb to fit negative binomial GLMMs.

32 glmer.nb

```
(gm1a <- glmer(cbind(incidence, size - incidence) ~ period + (1 | herd),
               cbpp, binomial, nAGQ = 9))
## GLMM with individual-level variability (accounting for overdispersion)
## For this data set the model is the same as one allowing for a period:herd
## interaction, which the plot indicates could be needed.
cbpp$obs <- 1:nrow(cbpp)</pre>
(gm2 <- glmer(cbind(incidence, size - incidence) ~ period +
    (1 | herd) + (1|obs),
              family = binomial, data = cbpp))
anova(gm1,gm2)
## glmer and glm log-likelihoods are consistent
gm1Devfun <- update(gm1,devFunOnly=TRUE)</pre>
gm0 <- glm(cbind(incidence, size - incidence) ~ period,</pre>
           family = binomial, data = cbpp)
## evaluate GLMM deviance at RE variance=theta=0, beta=(GLM coeffs)
gm1Dev0 <- gm1Devfun(c(0,coef(gm0)))</pre>
## compare
stopifnot(all.equal(gm1Dev0,c(-2*logLik(gm0))))
## the toenail oncholysis data from Backer et al 1998
## these data are notoriously difficult to fit
## Not run:
if (require("HSAUR2")) {
    gm2 <- glmer(outcome~treatment*visit+(1|patientID),</pre>
                 data=toenail,
                 family=binomial,nAGQ=20)
}
## End(Not run)
```

glmer.nb

Fitting Negative Binomial GLMMs

## Description

Fits a generalized linear mixed-effects model (GLMM) for the negative binomial family, building on glmer, and initializing via theta.ml from MASS.

# Usage

#### Arguments

... arguments as for glmer(.) such as formula, data, control, etc, but *not* family!

glmer.nb 33

interval	interval in which to start the optimization. The default is symmetric on log scale around the initially estimated theta.
tol	tolerance for the optimization via optimize.
verbose	logical indicating how much progress information should be printed during the optimization. Use verbose = 2 (or larger) to enable verbose=TRUE in the glmer() calls.
nb.control	<pre>optional list, like glmerControl(), used in refit(*, control = control.nb) during the optimization.</pre>
initCtrl	( <i>experimental</i> , <i>do not rely on this</i> :) a list with named components as in the default, passed to theta.ml (package MASS) for the initial value of the negative binomial parameter theta. May also include a theta component, in which case the initial estimation step is skipped

#### Value

An object of class glmerMod, for which many methods are available (e.g. methods(class="glmerMod")), see glmer.

#### Note

For historical reasons, the shape parameter of the negative binomial and the random effects parameters in our (G)LMM models are both called theta ( $\theta$ ), but are unrelated here.

The negative binomial  $\theta$  can be extracted from a fit g <- glmer.nb() by getME(g, "glmer.nb.theta").

Parts of glmer.nb() are still experimental and methods are still missing or suboptimal. In particular, there is no inference available for the dispersion parameter  $\theta$ , yet.

To fit a negative binomial model with *known* overdispersion parameter (e.g. as part of a model comparison exercise, use glmer with the negative.binomial family from the MASS package, e.g. glmer(...,family=MASS::negative.binomial(theta=1.75)).

#### See Also

glmer; from package MASS, negative.binomial (which we re-export currently) and theta.ml, the latter for initialization of optimization.

The 'Details' of pnbinom for the definition of the negative binomial distribution.

34 glmerLaplaceHandle

```
m.nb <- glmer.nb(y \sim f1*f2 + (1|g), data=dd, verbose=TRUE) m.nb ## The neg.binomial theta parameter: getME(m.nb, "glmer.nb.theta") LL <- logLik(m.nb) ## mixed model has 1 additional parameter (RE variance) stopifnot(attr(LL,"df")==attr(logLik(m.glm),"df")+1) plot(m.nb, resid(.) \sim g)# works, as long as data 'dd' is found ## End(Not run)
```

glmerLaplaceHandle

Handle for glmerLaplace

# Description

Handle for calling the glmerLaplace C++ function. Not intended for routine use.

# Usage

```
glmerLaplaceHandle(pp, resp, nAGQ, tol, maxit, verbose)
```

# **Arguments**

pp merPredD object
resp lmResp object
nAGQ see glmer
tol tolerance

maxit maximum number of pwrss iterations

verbose display optimizer progress

# Value

Value of the objective function

glmFamily 35

glmFamily

Generator object for the glmFamily class

# Description

The generator object for the glmFamily reference class. Such an object is primarily used through its new method.

## Usage

```
glmFamily(...)
```

## **Arguments**

... Named argument (see Note below)

#### Methods

```
new(family=family) Create a new glmFamily object
```

#### Note

Arguments to the new method must be named arguments.

## See Also

```
glmFamily
```

glmFamily-class

Class "glmFamily" - a reference class for family

# **Description**

This class is a wrapper class for family objects specifying a distibution family and link function for a generalized linear model (glm). The reference class contains an external pointer to a C++ object representing the class. For common families and link functions the functions in the family are implemented in compiled code so they can be accessed from other compiled code and for a speed boost.

#### **Extends**

All reference classes extend and inherit methods from "envRefClass".

36 golden-class

## Note

Objects from this reference class correspond to objects in a C++ class. Methods are invoked on the C++ class using the external pointer in the Ptr field. When saving such an object the external pointer is converted to a null pointer, which is why there is a redundant field ptr that is an active-binding function returning the external pointer. If the Ptr field is a null pointer, the external pointer is regenerated for the stored family field.

#### See Also

```
family, glmFamily
```

# **Examples**

```
str(glmFamily$new(family=poisson()))
```

golden-class

Class "golden" and Generator for Golden Search Optimizer Class

# **Description**

"golden" is a reference class for a golden search scalar optimizer, for a parameter within an interval. golden() is the generator for the "golden" class. The optimizer uses reverse communications.

# Usage

```
golden(...)
```

#### **Arguments**

... (partly optional) arguments passed to new() must be named arguments. lower and upper are the bounds for the scalar parameter; they must be finite.

## **Extends**

All reference classes extend and inherit methods from "envRefClass".

```
showClass("golden")
golden(lower= -100, upper= 1e100)
```

GQdk 37

GQdk

Sparse Gaussian / Gauss-Hermite Quadrature grid

## **Description**

Generate the sparse multidimensional Gaussian quadrature grids.

Currently unused. See GHrule() for the version currently in use in package lme4.

## Usage

```
GQdk(d = 1L, k = 1L)
GQN
```

## Arguments

d	integer scalar - the dimension of the function to be integrated with respect to the
	standard d-dimensional Gaussian density.

k integer scalar - the order of the grid. A grid of order k provides an exact result for a polynomial of total order of 2k - 1 or less.

## Value

GQdk() returns a matrix with d + 1 columns. The first column is the weights and the remaining d columns are the node coordinates.

GQN is a list of lists, containing the non-redundant quadrature nodes and weights for integration of a scalar function of a d-dimensional argument with respect to the density function of the d-dimensional Gaussian density function.

The outer list is indexed by the dimension, d, in the range of 1 to 20. The inner list is indexed by k, the order of the quadrature.

#### Note

GQN contains only the non-redundant nodes. To regenerate the whole array of nodes, all possible permutations of axes and all possible combinations of  $\pm 1$  must be applied to the axes. This entire array of nodes is exactly what GQdk() reproduces.

The number of nodes gets very large very quickly with increasing d and k. See the charts at <a href="http://www.sparse-grids.de">http://www.sparse-grids.de</a>.

```
GQdk(2,5) # 53 x 3
GQN[[3]][[5]] # a 14 x 4 matrix
```

38 grouseticks

grouseticks

Data on red grouse ticks from Elston et al. 2001

## Description

Number of ticks on the heads of red grouse chicks sampled in the field (grouseticks) and an aggregated version (grouseticks\_agg); see original source for more details

## Usage

```
data(grouseticks)
```

#### **Format**

```
INDEX (factor) chick number (observation level)
TICKS number of ticks sampled
BROOD (factor) brood number
HEIGHT height above sea level (meters)
YEAR year (-1900)
LOCATION (factor) geographic location code
CHEIGHT centered height, derived from HEIGHT
meanTICKS mean number of ticks by brood
varTICKS variance of number of ticks by brood
```

## **Details**

grouseticks\_agg is just a brood-level aggregation of the data

#### **Source**

Robert Moss, via David Elston

## References

Elston, D. A., R. Moss, T. Boulinier, C. Arrowsmith, and X. Lambin. 2001. "Analysis of Aggregation, a Worked Example: Numbers of Ticks on Red Grouse Chicks." Parasitology 122 (05): 563-569. doi:10.1017/S0031182001007740. http://journals.cambridge.org/action/displayAbstract? fromPage=online&aid=82701.

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## **Examples**

```
data(grouseticks)
## Figure 1a from Elston et al
par(las=1,bty="l")
tvec <- c(0,1,2,5,20,40,80)
pvec <- c(4,1,3)
with(grouseticks_agg,plot(1+meanTICKS~HEIGHT,
                  pch=pvec[factor(YEAR)],
                  log="y",axes=FALSE,
                  xlab="Altitude (m)",
                  ylab="Brood mean ticks"))
axis(side=1)
axis(side=2,at=tvec+1,label=tvec)
box()
abline(v=405,lty=2)
## Figure 1b
with(grouseticks_agg,plot(varTICKS~meanTICKS,
                  pch=4,
                  xlab="Brood mean ticks",
                  ylab="Within-brood variance"))
curve(1*x, from=0, to=70, add=TRUE)
## Model fitting
form <- TICKS~YEAR+HEIGHT+(1|BROOD)+(1|INDEX)+(1|LOCATION)</pre>
(full_mod1 <- glmer(form, family="poisson",data=grouseticks))</pre>
```

hatvalues.merMod

Diagonal elements of the hat matrix

## Description

Returns the values on the diagonal of the hat matrix, which is the matrix that transforms the response vector (minus any offset) into the fitted values (minus any offset). Note that this method should only be used for linear mixed models. It is not clear if the hat matrix concept even makes sense for generalized linear mixed models.

## Usage

```
## S3 method for class 'merMod'
hatvalues(model, fullHatMatrix = FALSE, ...)
```

## **Arguments**

```
model An object of class merMod.

fullHatMatrix Return full hat matrix (not just diagonal values)?

... Not currently used
```

#### Value

The diagonal elements of the hat matrix.

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#### **Examples**

```
m \leftarrow lmer(Reaction \sim Days + (Days \mid Subject), sleepstudy)
hatvalues(m)
```

InstEval

University Lecture/Instructor Evaluations by Students at ETH

## **Description**

University lecture evaluations by students at ETH Zurich, anonymized for privacy protection. This is an interesting "medium" sized example of a *partially* nested mixed effect model.

## **Format**

A data frame with 73421 observations on the following 7 variables.

- s a factor with levels 1:2972 denoting individual students.
- d a factor with 1128 levels from 1:2160, denoting individual professors or lecturers.
- studage an ordered factor with levels 2 < 4 < 6 < 8, denoting student's "age" measured in the *semester* number the student has been enrolled.
- lectage an ordered factor with 6 levels, 1 < 2 < ... < 6, measuring how many semesters back the lecture rated had taken place.
- service a binary factor with levels 0 and 1; a lecture is a "service", if held for a different department than the lecturer's main one.
- dept a factor with 14 levels from 1:15, using a random code for the department of the lecture.
- y a numeric vector of *ratings* of lectures by the students, using the discrete scale 1:5, with meanings of 'poor' to 'very good'.

Each observation is one student's rating for a specific lecture (of one lecturer, during one semester in the past).

#### **Details**

The main goal of the survey is to find "the best liked prof", according to the lectures given. Statistical analysis of such data has been the basis for a (student) jury selecting the final winners.

The present data set has been anonymized and slightly simplified on purpose.

```
str(InstEval)
head(InstEval, 16)
xtabs(~ service + dept, InstEval)
```

isNested 41

isNested

Is f1 nested within f2?

## **Description**

Does every level of f1 occur in conjunction with exactly one level of f2? The function is based on converting a triplet sparse matrix to a compressed column-oriented form in which the nesting can be quickly evaluated.

## Usage

```
isNested(f1, f2)
```

## **Arguments**

```
f1 factor 1
f2 factor 2
```

## Value

TRUE if factor 1 is nested within factor 2

## **Examples**

```
with(Pastes, isNested(cask, batch)) ## => FALSE
with(Pastes, isNested(sample, batch)) ## => TRUE
```

isREML

Check characteristics of models

## Description

Check characteristics of models: whether a model fit corresponds to a linear (LMM), generalized linear (GLMM), or nonlinear (NLMM) mixed model, and whether a linear mixed model has been fitted by REML or not (i sREML(x) is always FALSE for GLMMs and NLMMs).

## Usage

```
isREML(x, ...)
isLMM(x, ...)
isNLMM(x, ...)
isGLMM(x, ...)
```

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## Arguments

x a fitted model.

... additional, optional arguments. (None are used in the merMod methods)

#### **Details**

These are generic functions. At present the only methods are for mixed-effects models of class merMod.

#### Value

a logical value

#### See Also

getME

## **Examples**

lmer

Fit Linear Mixed-Effects Models

## **Description**

Fit a linear mixed-effects model (LMM) to data, via REML or maximum likelihood.

## Usage

```
lmer(formula, data = NULL, REML = TRUE, control = lmerControl(),
    start = NULL, verbose = 0L, subset, weights, na.action,
    offset, contrasts = NULL, devFunOnly = FALSE, ...)
```

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#### **Arguments**

formula

a two-sided linear formula object describing both the fixed-effects and random-effects part of the model, with the response on the left of a ~ operator and the terms, separated by + operators, on the right. Random-effects terms are distinguished by vertical bars (|) separating expressions for design matrices from grouping factors. Two vertical bars (||) can be used to specify multiple uncorrelated random effects for the same grouping variable. (Because of the way it is implemented, the ||-syntax works only for design matrices containing numeric (continuous) predictors; to fit models with independent categorical effects, see dummy or the lmer\_alt function from the afex package.)

data

an optional data frame containing the variables named in formula. By default the variables are taken from the environment from which lmer is called. While data is optional, the package authors *strongly* recommend its use, especially when later applying methods such as update and drop1 to the fitted model (*such methods are not guaranteed to work properly if* data *is omitted*). If data is omitted, variables will be taken from the environment of formula (if specified as a formula) or from the parent frame (if specified as a character vector).

REML

logical scalar - Should the estimates be chosen to optimize the REML criterion (as opposed to the log-likelihood)?

control

a list (of correct class, resulting from lmerControl() or glmerControl() respectively) containing control parameters, including the nonlinear optimizer to be used and parameters to be passed through to the nonlinear optimizer, see the \*lmerControl documentation for details.

start

a named list of starting values for the parameters in the model. For lmer this can be a numeric vector or a list with one component named "theta".

verbose

integer scalar. If > 0 verbose output is generated during the optimization of the parameter estimates. If > 1 verbose output is generated during the individual PIRLS steps.

subset

an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.

weights

an optional vector of 'prior weights' to be used in the fitting process. Should be NULL or a numeric vector. Prior weights are *not* normalized or standardized in any way. In particular, the diagonal of the residual covariance matrix is the squared residual standard deviation parameter sigma times the vector of inverse weights. Therefore, if the weights have relatively large magnitudes, then in order to compensate, the sigma parameter will also need to have a relatively large magnitude.

na.action

a function that indicates what should happen when the data contain NAs. The default action (na.omit, inherited from the 'factory fresh' value of getOption("na.action")) strips any observations with any missing values in any variables.

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

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formula instead or as well, and if more than one is specified their sum is used. See model.offset.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

devFun0nly logical - return only the deviance evaluation function. Note that because the

deviance function operates on variables stored in its environment, it may not return *exactly* the same values on subsequent calls (but the results should always

be within machine tolerance).

other potential arguments. A method argument was used in earlier versions of

the package. Its functionality has been replaced by the REML argument.

#### Details

• If the formula argument is specified as a character vector, the function will attempt to coerce it to a formula. However, this is not recommended (users who want to construct formulas by pasting together components are advised to use as.formula or reformulate); model fits will work but subsequent methods such as drop1, update may fail.

- When handling perfectly collinear predictor variables (i.e. design matrices of less than full rank), [gn]lmer is not quite as sophisticated as some simpler modeling frameworks such as lm and glm. While it does automatically drop collinear variables (with a message rather than a warning), it does not automatically fill in NA values for the dropped coefficients; these can be added via fixef(fitted.model,add.dropped=TRUE). This information can also be retrieved via attr(getME(fitted.model,"X"), "col.dropped").
- the deviance function returned when devFunOnly is TRUE takes a single numeric vector argument, representing the theta vector. This vector defines the scaled variance-covariance matrices of the random effects, in the Cholesky parameterization. For models with only simple (intercept-only) random effects, theta is a vector of the standard deviations of the random effects. For more complex or multiple random effects, running getME(.,"theta") to retrieve the theta vector for a fitted model and examining the names of the vector is probably the easiest way to determine the correspondence between the elements of the theta vector and elements of the lower triangles of the Cholesky factors of the random effects.

#### Value

An object of class merMod (more specifically, an object of *subclass* lmerMod), for which many methods are available (e.g. methods(class="merMod"))

#### See Also

lm for linear models; glmer for generalized linear; and nlmer for nonlinear mixed models.

```
## linear mixed models - reference values from older code
(fm1 <- lmer(Reaction ~ Days + (Days | Subject), sleepstudy))
summary(fm1)# (with its own print method; see class?merMod % ./merMod-class.Rd
str(terms(fm1))
stopifnot(identical(terms(fm1, fixed.only=FALSE),</pre>
```

```
terms(model.frame(fm1))))
attr(terms(fm1, FALSE), "dataClasses") # fixed.only=FALSE needed for dataCl.
fm1_ML <- update(fm1,REML=FALSE)</pre>
(fm2 <- lmer(Reaction ~ Days + (Days || Subject), sleepstudy))</pre>
anova(fm1, fm2)
sm2 <- summary(fm2)</pre>
print(fm2, digits=7, ranef.comp="Var") # the print.merMod()
                                                                       method
print(sm2, digits=3, corr=FALSE)
                                        # the print.summary.merMod() method
(vv <- vcov.merMod(fm2, corr=TRUE))</pre>
as(vv, "corMatrix")# extracts the ("hidden") 'correlation' entry in @factors
## Fit sex-specific variances by constructing numeric dummy variables
## for sex and sex:age; in this case the estimated variance differences
## between groups in both intercept and slope are zero ...
data(Orthodont,package="nlme")
Orthodont$nsex <- as.numeric(Orthodont$Sex=="Male")</pre>
Orthodont$nsexage <- with(Orthodont, nsex*age)
lmer(distance ~ age + (age|Subject) + (0+nsex|Subject) +
     (0 + nsexage|Subject), data=Orthodont)
```

lmerControl

Control of Mixed Model Fitting

## **Description**

Construct control structures for mixed model fitting. All arguments have defaults, and can be grouped into

- general control parameters, most importantly optimizer, further restart\_edge, etc;
- model- or data-checking specifications, in short "checking options", such as check.nobs.vs.rankZ, or check.rankX (currently not for nlmerControl);
- all the parameters to be passed to the optimizer, e.g., maximal number of iterations, passed via the optCtrl list argument.

## Usage

```
lmerControl(optimizer = "bobyqa",
    restart_edge = TRUE,
    boundary.tol = 1e-5,
    calc.derivs=TRUE,
    use.last.params=FALSE,
    sparseX = FALSE,
    ## input checking options
    check.nobs.vs.rankZ = "ignore",
    check.nobs.vs.nlev = "stop",
    check.nlev.gtreq.5 = "ignore",
```

```
check.nlev.gtr.1 = "stop",
    check.nobs.vs.nRE="stop",
    check.rankX = c("message+drop.cols", "silent.drop.cols", "warn+drop.cols",
                    "stop.deficient", "ignore"),
   check.scaleX = c("warning","stop","silent.rescale",
                              "message+rescale", "warn+rescale", "ignore"),
   check.formula.LHS = "stop",
    ## convergence checking options
   check.conv.grad = .makeCC("warning", tol = 2e-3, relTol = NULL),
   check.conv.singular = .makeCC(action = "ignore", tol = 1e-4),
    check.conv.hess
                       = .makeCC(action = "warning", tol = 1e-6),
    ## optimizer args
   optCtrl = list())
glmerControl(optimizer = c("bobyqa", "Nelder_Mead"),
    restart_edge = FALSE,
   boundary.tol = 1e-5,
    calc.derivs=TRUE,
   use.last.params=FALSE,
    sparseX = FALSE,
   tolPwrss=1e-7,
   compDev=TRUE,
   nAGQ0initStep=TRUE,
   ## input checking options
   check.nobs.vs.rankZ = "ignore",
   check.nobs.vs.nlev = "stop",
    check.nlev.gtreq.5 = "ignore",
    check.nlev.gtr.1 = "stop",
    check.nobs.vs.nRE="stop",
    check.rankX = c("message+drop.cols", "silent.drop.cols", "warn+drop.cols",
                    "stop.deficient", "ignore"),
   check.scaleX = "warning",
    check.formula.LHS = "stop",
    check.response.not.const = "stop",
    ## convergence checking options
   check.conv.grad
                       = .makeCC("warning", tol = 1e-3, relTol = NULL),
    check.conv.singular = .makeCC(action = "ignore", tol = 1e-4),
                       = .makeCC(action = "warning", tol = 1e-6),
    check.conv.hess
    ## optimizer args
   optCtrl = list())
nlmerControl(optimizer = "Nelder_Mead", tolPwrss = 1e-10,
            optCtrl = list())
.makeCC(action, tol, relTol, ...)
```

## **Arguments**

optimizer

character - name of optimizing function(s). A character vector or list of functions: length 1 for 1mer or glmer, possibly length 2 for glmer). The built-in optimizers are Nelder\_Mead and bobyqa (from the minqa package). Any minimizing function that allows box constraints can be used provided that it

- (1) takes input parameters fn (function to be optimized), par (starting parameter values), lower and upper (parameter bounds) and control (control parameters, passed through from the control argument) and
- (2) returns a list with (at least) elements par (best-fit parameters), fval (best-fit function value), conv (convergence code, equal to zero for successful convergence) and (optionally) message (informational message, or explanation of convergence failure).

Special provisions are made for bobyga, Nelder\_Mead, and optimizers wrapped in the optimx package; to use the optimx optimizers (including L-BFGS-B from base optim and nlminb), pass the method argument to optim in the optCtrl argument (you may also need to load the optimx package manually using library(optimx) or require(optimx)).

For glmer, if length(optimizer)==2, the first element will be used for the preliminary (random effects parameters only) optimization, while the second will be used for the final (random effects plus fixed effect parameters) phase. See modular for more information on these two phases.

If optimizer is NULL (at present for 1mer only), all of the model structures will be set up, but no optimization will be done (e.g. parameters will all be returned as NA).

calc.derivs use.last.params

logical - compute gradient and Hessian of nonlinear optimization solution?

logical - should the last value of the parameters evaluated (TRUE), rather than the value of the parameters corresponding to the minimum deviance, be returned? This is a "backward bug-compatibility" option; use TRUE only when trying to match previous results.

sparseX logical - should a sparse model matrix be used for the fixed-effects terms? Currently inactive.

> logical - should the optimizer attempt a restart when it finds a solution at the boundary (i.e. zero random-effect variances or perfect +/-1 correlations)? (Currently only implemented for lmerControl.)

boundary.tol numeric - within what distance of a boundary should the boundary be checked for a better fit? (Set to zero to disable boundary checking.)

> numeric scalar - the tolerance for declaring convergence in the penalized iteratively weighted residual sum-of-squares step.

> logical scalar - should compiled code be used for the deviance evaluation during the optimization of the parameter estimates?

> Run an initial optimization phase with nAGQ = 0. While the initial optimization usually provides a good starting point for subsequent fitting (thus increasing overall computational speed), setting this option to FALSE can be useful in cases where the initial phase results in bad fixed-effect estimates (seen most often in binomial models with link="cloglog" and offsets).

restart\_edge

tolPwrss

compDev

nAGQ0initStep

check.nlev.gtreq.5

character - rules for checking whether all random effects have  $\geq$  5 levels. See action.

check.nlev.gtr.1

character - rules for checking whether all random effects have > 1 level. See action.

check.nobs.vs.rankZ

character - rules for checking whether the number of observations is greater than (or greater than or equal to) the rank of the random effects design matrix (Z), usually necessary for identifiable variances. As for action, with the addition of "warningSmall" and "stopSmall", which run the test only if the dimensions of Z are < le6. nobs > rank(Z) will be tested for LMMs and GLMMs with estimated scale parameters; nobs >= rank(Z) will be tested for GLMMs with fixed scale parameter. The rank test is done using the method="qr" option of the rankMatrix function.

check.nobs.vs.nlev

character - rules for checking whether the number of observations is less than (or less than or equal to) the number of levels of every grouping factor, usually necessary for identifiable variances. As for action. nobs<nlevels will be tested for LMMs and GLMMs with estimated scale parameters; nobs<=nlevels will be tested for GLMMs with fixed scale parameter.

check.nobs.vs.nRE

character - rules for checking whether the number of observations is greater than (or greater than or equal to) the number of random-effects levels for each term, usually necessary for identifiable variances. As for check.nobs.vs.nlev.

check.conv.grad

rules for checking the gradient of the deviance function for convergence. A list as returned by .makeCC, or a character string with only the action.

check.conv.singular

rules for checking for a singular fit, i.e. one where some parameters are on the boundary of the feasible space (for example, random effects variances equal to 0 or correlations between random effects equal to  $\pm 1.0$ ); as for check.conv.grad above.

check.conv.hess

rules for checking the Hessian of the deviance function for convergence.; as for check.conv.grad above.

check.rankX

character - specifying if rankMatrix(X) should be compared with ncol(X) and if columns from the design matrix should possibly be dropped to ensure that it has full rank. Sometimes needed to make the model identifiable. The options can be abbreviated; the three "\*.drop.cols" options all do drop columns, "stop.deficient" gives an error when the rank is smaller than the number of columns where "ignore" does no rank computation, and will typically lead to less easily understandable errors, later.

check.scaleX character - check for problematic scaling of columns of fixed-effect model matrix, e.g. parameters measured on very different scales.

check.formula.LHS

check whether specified formula has a left-hand side. Primarily for internal use

within simulate.merMod; use at your own risk as it may allow the generation of unstable merMod objects

check.response.not.const

character - check that the response is not constant.

optCtrl a list of additional arguments to be passed to the nonlinear optimizer (see

Nelder\_Mead, bobyqa). In particular, both Nelder\_Mead and bobyqa use maxfun to specify the maximum number of function evaluations they will try before giving up - in contrast to optim and optimx-wrapped optimizers, which use maxit.

action character - generic choices for the severity level of any test. "ignore": skip the

test. "warning": warn if test fails. "stop": throw an error if test fails.

tol numeric - tolerance for check

relTol numeric - tolerance for checking relative variation
... other elements to include in check specification

#### **Details**

Note that (only!) the pre-fitting "checking options" (i.e., all those starting with "check." but *not* including the convergence checks ("check.conv.\*") or rank-checking ("check.rank\*") options) may also be set globally via options. In that case, (g)lmerControl will use them rather than the default values, but will *not* override values that are passed as explicit arguments.

For example, options(lmerControl=list(check.nobs.vs.rankZ = "ignore")) will suppress warnings that the number of observations is less than the rank of the random effects model matrix Z.

## Value

The \*Control functions return a list (inheriting from class "merControl") containing

- 1. general control parameters, such as optimizer, restart\_edge;
- 2. (currently not for nlmerControl:) "checkControl", a list of data-checking specifications, e.g., check.nobs.vs.rankZ;
- 3. parameters to be passed to the optimizer, i.e., the optCtrl list, which may contain maxiter.

.makeCC returns a list containing the check specification (action, tolerance, and optionally relative tolerance).

## See Also

convergence

```
str(lmerControl())
str(glmerControl())
## Not run:
    ## fit with default "bobyqa" algorithm ...
fm0 <- lmer(Reaction ~ Days + (1 | Subject), sleepstudy)
fm1 <- lmer(Reaction ~ Days + (Days | Subject), sleepstudy)</pre>
```

```
## or with "Nelder_Mead" (the previous default) ...
    fm1_bobyqa <- update(fm1, control = lmerControl(optimizer="Nelder_Mead"))</pre>
    ## or with the nlminb function used in older (<1.0) versions of lme4;
    ## this will usually replicate older results
    require(optimx)
    fm1_nlminb <- update(fm1,</pre>
                     control = lmerControl(optimizer= "optimx",
                                            optCtrl = list(method="nlminb")))
    ## The other option here is method="L-BFGS-B".
    ## Or we can wrap base::optim():
    optimwrap <- function(fn,par,lower,upper,control=list(),</pre>
                           ...) {
        if (is.null(control$method)) stop("must specify method in optCtrl")
        method <- control$method</pre>
        control$method <- NULL</pre>
        ## "Brent" requires finite upper values (lower bound will always
        ## be zero in this case)
        if (method=="Brent") upper <- pmin(1e4,upper)</pre>
        res <- optim(par=par, fn=fn, lower=lower,upper=upper,</pre>
                     control=control, method=method, ...)
        with(res, list(par = par,
                        fval = value,
                        feval= counts[1],
                       conv = convergence,
                        message = message))
    fm0_brent <- update(fm0,</pre>
                   control = lmerControl(optimizer = "optimwrap",
                                           optCtrl = list(method="Brent")))
    ## You can also use functions from the nloptr package.
    if (require(nloptr)) {
        defaultControl <- list(algorithm="NLOPT_LN_BOBYQA",</pre>
                                xtol_abs=1e-6,ftol_abs=1e-6,maxeval=1e5)
        nloptwrap <- function(fn,par,lower,upper,control=list(),...) {</pre>
            for (n in names(defaultControl))
                if (is.null(control[[n]])) control[[n]] <- defaultControl[[n]]</pre>
            res <- nloptr(x0=par,eval_f=fn,lb=lower,ub=upper,opts=control,...)</pre>
            with(res, list(par = solution,
                            fval = objective,
                            feval= iterations,
                            conv = if (status>0) 0 else status,
                            message = message))
        fm1_nloptr
                      <- update(fm1, control=lmerControl(optimizer="nloptwrap"))</pre>
        fm1_nloptr_NM <- update(fm1, control=lmerControl(optimizer="nloptwrap",</pre>
                                         optCtrl=list(algorithm="NLOPT_LN_NELDERMEAD")))
    ## other algorithm options include NLOPT_LN_COBYLA, NLOPT_LN_SBPLX
## End(Not run)
```

lmList 51

lmList	Fit List of lm or glm Objects with a Common Model	

# Description

Fit a list of 1m or g1m objects with a common model for different subgroups of the data.

# Usage

## Arguments

formula	a linear formula object of the form $y \sim x1++xn \mid g$ . In the formula object, y represents the response, $x1,,xn$ the covariates, and g the grouping factor specifying the partitioning of the data according to which different 1m fits should be performed.
family	an optional family specification for a generalized linear model (glm).
data	an optional data frame containing the variables named in formula. By default the variables are taken from the environment from which 1mer is called. See Details.
subset	an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.
weights	an optional vector of 'prior weights' to be used in the fitting process. Should be NULL or a numeric vector.
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.omit, inherited from the 'factory fresh' value of getOption("na.action")) strips any observations with any missing values in any variables.
offset	this can be used to specify an <i>a priori</i> 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.
pool	logical scalar, should the variance estimate pool the residual sums of squares
warn	indicating if errors in the single fits should signal a "summary" warning.
	additional, optional arguments to be passed to the model function or family evaluation.

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#### **Details**

- While data is optional, the package authors *strongly* recommend its use, especially when later applying methods such as update and drop1 to the fitted model (*such methods are not guaranteed to work properly if data is omitted*). If data is omitted, variables will be taken from the environment of formula (if specified as a formula) or from the parent frame (if specified as a character vector).
- Since **lme4** version 1.1-16, if there are errors (see stop) in the single (lm() or glm()) fits, they are summarized to a warning message which is returned as attribute "warnMessage" and signalled as warning() when the warn argument is true.

In previous **lme4** versions, a general (different) warning had been signalled in this case.

#### Value

an object of class lmList4 (see there, notably for the methods defined).

#### See Also

1mList4

## **Examples**

```
fm.plm <- lmList(Reaction ~ Days | Subject, sleepstudy)
coef(fm.plm)
fm.2 <- update(fm.plm, pool = FALSE)
## coefficients are the same, "pooled or unpooled":
stopifnot( all.equal(coef(fm.2), coef(fm.plm)) )

(ci <- confint(fm.plm)) # print and rather *see* :
plot(ci) # how widely they vary for the individuals</pre>
```

lmList4-class

Class "lmList4" of 'lm' Objects on Common Model

## **Description**

Class "lmList4" is an S4 class with basically a list of objects of class lm with a common model (but different data); see lmList() which returns these.

Package **nlme**'s lmList() returns objects of S3 class "lmList" and provides methods for them, on which our methods partly build.

## **Objects from the Class**

Objects can be created by calls of the form new("lmList4", ...) or, more commonly, by a call to lmList().

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## Methods

A dozen methods are provided. Currently, S4 methods for show, coercion (as(.,.)) and others inherited via "list", and S3 methods for coef, confint, fitted, fixef, formula, logLik, pairs, plot, predict, print, qqnorm, ranef, residuals, sigma, summary, and update.

**sigma(object)** returns the standard deviation  $\hat{\sigma}$  (of the errors in the linear models), assuming a *common* variance  $\sigma^2$  by pooling (even when pool = FALSE was used in the fit).

#### See Also

1mList

## **Examples**

```
if(getRversion() >= "3.2.0") {
   (mm <- methods(class = "lmList4"))
   ## The S3 ("not S4") ones :
    mm[!attr(mm,"info")[,"isS4"]]
}
## For more examples: example(lmList) i.e., ?lmList</pre>
```

1mResp

Generator objects for the response classes

## **Description**

The generator objects for the lmResp, lmerResp, glmResp and nlsResp reference classes. Such objects are primarily used through their new methods.

## Usage

```
lmResp(...)
```

## **Arguments**

... List of arguments (see Note).

## Methods

```
new(y=y): Create a new lmResp or lmerResp object.
new(family=family, y=y): Create a new glmResp object.
new(y=y, nlmod=nlmod, nlenv=nlenv, pnames=pnames, gam=gam): Create a new nlsResp object.
```

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#### Note

Arguments to the new methods must be named arguments.

- y the numeric response vector
- family a family object
- · nlmod the nonlinear model function
- nlenv an environment holding data objects for evaluation of nlmod
- pnames a character vector of parameter names
- gam a numeric vector the initial linear predictor

#### See Also

lmResp, lmerResp, glmResp, nlsResp

lmResp-class	Reference	Classes	for	Response	Modules,
	"(lm glm nl	s lmer)Resp"			

## **Description**

Reference classes for response modules, including linear models, "lmResp", generalized linear models, "glmResp", nonlinear models, "nlsResp" and linear mixed-effects models, "lmerResp". Each reference class is associated with a C++ class of the same name. As is customary, the generator object for each class has the same name as the class.

#### Extends

All reference classes extend and inherit methods from "envRefClass". Furthermore, "glmResp", "nlsResp" and "lmerResp" all extend the "lmResp" class.

#### Note

Objects from these reference classes correspond to objects in C++ classes. Methods are invoked on the C++ classes using the external pointer in the ptr field. When saving such an object the external pointer is converted to a null pointer, which is why there are redundant fields containing enough information as R objects to be able to regenerate the C++ object. The convention is that a field whose name begins with an upper-case letter is an R object and the corresponding field whose name begins with the lower-case letter is a method. Access to the external pointer should be through the method, not through the field.

#### See Also

lmer, glmer, nlmer, merMod.

## **Examples**

```
showClass("lmResp")
str(lmResp$new(y=1:4))
showClass("glmResp")
str(glmResp$new(family=poisson(), y=1:4))
showClass("nlsResp")
showClass("lmerResp")
str(lmerResp$new(y=1:4))
```

merMod-class

Class "merMod" of Fitted Mixed-Effect Models

## **Description**

A mixed-effects model is represented as a merPredD object and a response module of a class that inherits from class lmResp. A model with a lmerResp response has class lmerMod; a glmResp response has class glmerMod; and a nlsResp response has class nlmerMod.

## Usage

```
## S3 method for class 'merMod'
anova(object, ..., refit = TRUE, model.names=NULL)
## S3 method for class 'merMod'
as.function(x, ...)
## S3 method for class 'merMod'
coef(object, ...)
## S3 method for class 'merMod'
deviance(object, REML = NULL, ...)
REMLcrit(object)
## S3 method for class 'merMod'
extractAIC(fit, scale = 0, k = 2, ...)
## S3 method for class 'merMod'
family(object, ...)
## S3 method for class 'merMod'
formula(x, fixed.only = FALSE, random.only = FALSE, ...)
## S3 method for class 'merMod'
fitted(object, ...)
## S3 method for class 'merMod'
logLik(object, REML = NULL, ...)
## S3 method for class 'merMod'
nobs(object, ...)
## S3 method for class 'merMod'
ngrps(object, ...)
## S3 method for class 'merMod'
terms(x, fixed.only = TRUE, random.only = FALSE, ...)
## S3 method for class 'merMod'
vcov(object, correlation = TRUE, sigm = sigma(object),
```

```
use.hessian = NULL, ...)
## S3 method for class 'merMod'
model.frame(formula, fixed.only = FALSE, ...)
## S3 method for class 'merMod'
model.matrix(object, type = c("fixed", "random", "randomListRaw"), ...)
## S3 method for class 'merMod'
print(x, digits = max(3, getOption("digits") - 3),
     correlation = NULL, symbolic.cor = FALSE,
     signif.stars = getOption("show.signif.stars"), ranef.comp = "Std.Dev.", ...)
## S3 method for class 'merMod'
summary(object, correlation = , use.hessian = NULL, ...)
## S3 method for class 'summary.merMod'
print(x, digits = max(3, getOption("digits") - 3),
     correlation = NULL, symbolic.cor = FALSE,
     signif.stars = getOption("show.signif.stars"),
     ranef.comp = c("Variance", "Std.Dev."), show.resids = TRUE, ...)
## S3 method for class 'merMod'
update(object, formula., ..., evaluate = TRUE)
## S3 method for class 'merMod'
weights(object, type = c("prior", "working"), ...)
```

#### **Arguments**

object an R object of class merMod, i.e., as resulting from lmer(), or glmer(), etc.

x an R object of class merMod or summary.merMod, respectively, the latter result-

ing from summary(<merMod>).

fit an R object of class merMod.

formula in the case of model.frame, a merMod object.

refit logical indicating if objects of class 1merMod should be refitted with ML before

comparing models. The default is TRUE to prevent the common mistake of inappropriately comparing REML-fitted models with different fixed effects, whose

likelihoods are not directly comparable.

model.names character vectors of model names to be used in the anova table.

scale Not currently used (see extractAIC).

k see extractAIC.

REML Logical. If TRUE, return the restricted log-likelihood rather than the log-likelihood.

If NULL (the default), set REML to isREML(object) (see isREML).

fixed.only logical indicating if only the fixed effects components (terms or formula ele-

ments) are sought. If false, all components, including random ones, are returned.

random.only complement of fixed.only; indicates whether random components only are

sought. (Trying to specify fixed.only and random.only at the same time will

produce an error.)

correlation (logical) for vcov, indicates whether the correlation matrix as well as the variance-

covariance matrix is desired; for summary.merMod, indicates whether the correlation matrix should be computed and stored along with the covariance; for

> print.summary.merMod, indicates whether the correlation matrix of the fixedeffects parameters should be printed. In the latter case, when NULL (the default), the correlation matrix is printed when it has been computed by summary(.), and when  $p \le 20$ .

use hessian

(logical) indicates whether to use the finite-difference Hessian of the deviance function to compute standard errors of the fixed effects, rather estimating based on internal information about the inverse of the model matrix (see getME(., "RX")). The default is to to use the Hessian whenever the fixed effect parameters are arguments to the deviance function (i.e. for GLMMs with nAGQ>0), and to use getME(., "RX") whenever the fixed effect parameters are profiled out (i.e. for GLMMs with nAGQ==0 or LMMs).

use.hessian=FALSE is backward-compatible with older versions of lme4, but may give less accurate SE estimates when the estimates of the fixed-effect (see getME(., "beta")) and random-effect (see getME(., "theta")) parameters are

correlated.

the residual standard error; by default sigma(object). sigm

digits number of significant digits for printing

should a symbolic encoding of the fixed-effects correlation matrix be printed? symbolic.cor

If so, the symnum function is used.

signif.stars (logical) should significance stars be used?

ranef.comp character vector of length one or two, indicating if random-effects parameters

should be reported on the variance and/or standard deviation scale.

show.resids should the quantiles of the scaled residuals be printed?

formula. see update.formula.

evaluate see update.

For weights, type of weights to be returned; either "prior" for the initially type

> supplied weights or "working" for the weights at the final iteration of the penalized iteratively reweighted least squares algorithm. For model.matrix, type of model matrix to return (one of fixed giving the fixed effects model matrix, random giving the random effects model matrix, or randomListRaw giving a list of the raw random effects model matrices associated with each random effects

term).

potentially further arguments passed from other methods.

#### **Objects from the Class**

Objects of class merMod are created by calls to lmer, glmer or nlmer.

## S3 methods

The following S3 methods with arguments given above exist (this list is currently not complete):

anova: returns the sequential decomposition of the contributions of fixed-effects terms or, for multiple arguments, model comparison statistics. For objects of class 1merMod the default behavior is to refit the models with ML if fitted with REML = TRUE, this can be controlled via the refit argument. See also anova.

as.function: returns the deviance function, the same as lmer(\*, devFunOnly=TRUE), and mkLmerDevfun() or mkGlmerDevfun(), respectively.

coef: Computes the sum of the random and fixed effects coefficients for each explanatory variable for each level of each grouping factor.

extractAIC: Computes the (generalized) Akaike An Information Criterion. If isREML(fit), then fit is refitted using maximum likelihood.

family: family of fitted GLMM. (*Warning:* this accessor may not work properly with customized families/link functions.)

fitted: Fitted values, given the conditional modes of the random effects. For more flexible access to fitted values, use predict.merMod.

logLik: Log-likelihood at the fitted value of the parameters. Note that for GLMMs, the returned value is only proportional to the log probability density (or distribution) of the response variable. See logLik.

model.frame: returns the frame slot of merMod.

model.matrix: returns the fixed effects model matrix.

nobs, ngrps: Number of observations and vector of the numbers of levels in each grouping factor. See ngrps.

summary: Computes and returns a list of summary statistics of the fitted model, the amount of output can be controlled via the print method, see also summary.

print.summary: Controls the output for the summary method.

vcov: Calculate variance-covariance matrix of the *fixed* effect terms, see also vcov.

update: See update.

## Deviance and log-likelihood of GLMMs

One must be careful when defining the deviance of a GLM. For example, should the deviance be defined as minus twice the log-likelihood or does it involve subtracting the deviance for a saturated model? To distinguish these two possibilities we refer to absolute deviance (minus twice the log-likelihood) and relative deviance (relative to a saturated model, e.g. Section 2.3.1 in McCullagh and Nelder 1989). With GLMMs however, there is an additional complication involving the distinction between the likelihood and the conditional likelihood. The latter is the likelihood obtained by conditioning on the estimates of the conditional modes of the spherical random effects coefficients, whereas the likelihood itself (i.e. the unconditional likelihood) involves integrating out these coefficients. The following table summarizes how to extract the various types of deviance for a glmerMod object:

```
conditional unconditional relative deviance(object) NA in lme4 absolute object@resp$aic() -2*logLik(object)
```

This table requires two caveats:

• If the link function involves a scale parameter (e.g. Gamma) then object@resp\$aic() - 2 \* getME(object, is required for the absolute-conditional case.

"devc

• If adaptive Gauss-Hermite quadrature is used, then logLik(object) is currently only proportional to the absolute-unconditional log-likelihood.

For more information about this topic see the misc/logLikGLMM directory in the package source.

#### **Slots**

```
resp: A reference class object for an Ime4 response module (1mResp-class).

Gp: See getME.

call: The matched call.

frame: The model frame containing all of the variables required to parse the model formula.

flist: See getME.

cnms: See getME.

lower: See getME.

theta: Covariance parameter vector.

beta: Fixed effects coefficients.

u: Conditional model of spherical random effects coefficients.

devcomp: See getME.

pp: A reference class object for an Ime4 predictor module (merPredD-class).

optinfo: List containing information about the nonlinear optimization.
```

## See Also

```
lmer, glmer, nlmer, merPredD, lmerResp, glmResp, nlsResp
```

Other methods for merMod objects documented elsewhere include: fortify.merMod, drop1.merMod, isLMM.merMod, isGLMM.merMod, isNLMM.merMod, isREML.merMod, plot.merMod, predict.merMod, profile.merMod, ranef.merMod, refit.merMod, refitML.merMod, residuals.merMod, sigma.merMod, simulate.merMod, summary.merMod.

```
showClass("merMod")
methods(class="merMod")## over 30 (S3) methods available
## -> example(lmer) for an example of vcov.merMod()
```

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merPredD

Generator object for the merPredD class

## **Description**

The generator object for the merPredD reference class. Such an object is primarily used through its new method.

#### Usage

```
merPredD(...)
```

## **Arguments**

... List of arguments (see Note).

#### Note

```
merPredD(...) is a short form of new("merPredD", ...) to create a new merPredD object and the ... must be named arguments, (X, Zt, Lambdat, Lind, theta,n):
```

X: dense model matrix for the fixed-effects parameters, to be stored in the X field.

Zt: transpose of the sparse model matrix for the random effects. It is stored in the Zt field.

Lambdat: transpose of the sparse lower triangular relative variance factor (stored in the Lambdat field).

Lind: integer vector of the same length as the x slot in the Lambdat field. Its elements should be in the range 1 to the length of the theta field.

theta: numeric vector of variance component parameters (stored in the theta field).

n: sample size, usually nrow(X).

## See Also

The class definition, merPredD, also for examples.

merPredD-class

Class "merPredD" - a Dense Predictor Reference Class

## **Description**

A reference class (see mother class definition "envRefClass" for a mixed-effects model predictor module with a dense model matrix for the fixed-effects parameters. The reference class is associated with a C++ class of the same name. As is customary, the generator object, merPredD, for the class has the same name as the class.

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#### Note

Objects from this reference class correspond to objects in a C++ class. Methods are invoked on the C++ class object using the external pointer in the Ptr field. When saving such an object the external pointer is converted to a null pointer, which is why there are redundant fields containing enough information as R objects to be able to regenerate the C++ object. The convention is that a field whose name begins with an upper-case letter is an R object and the corresponding field, whose name begins with the lower-case letter is a method. References to the external pointer should be through the method, not directly through the Ptr field.

#### See Also

```
lmer, glmer, nlmer, merPredD, merMod.
```

#### **Examples**

```
showClass("merPredD")
pp <- slot(lmer(Yield ~ 1|Batch, Dyestuff), "pp")
stopifnot(is(pp, "merPredD"))
str(pp) # an overview of all fields and methods' names.</pre>
```

mkMerMod

Create a 'merMod' Object

## Description

Create an object of (a subclass of) class merMod from the environment of the objective function and the value returned by the optimizer.

## Usage

```
mkMerMod(rho, opt, reTrms, fr, mc, lme4conv = NULL)
```

## Arguments

rho	the environment of the objective function
opt	the optimization result returned by the optimizer (a list: see $lmerControl$ for required elements)
reTrms	random effects structure from the calling function (see $mkReTrms$ for required elements)
fr	model frame (see model.frame)
mc	matched call from the calling function
lme4conv	lme4-specific convergence information (results of checkConv)

#### Value

an object from a class that inherits from merMod.

62 mkReTrms

mkRespMod	Create an lmerResp, glmResp or nlsResp instance	

## **Description**

Create an ImerResp, glmResp or nlsResp instance

## Usage

```
mkRespMod(fr, REML = NULL, family = NULL, nlenv = NULL,
nlmod = NULL, ...)
```

## **Arguments**

fr	a model frame
REML	logical scalar, value of REML for an ImerResp instance
family	the optional glm family (glmResp only)
nlenv	the nonlinear model evaluation environment (nlsResp only)
nlmod	the nonlinear model function (nlsResp only)
•••	where to look for response information if fr is missing. Can contain a model response, y, offset, offset, and weights, weights.

## Value

an ImerResp or glmResp or nlsResp instance

## See Also

Other utilities: findbars, mkReTrms, nlformula, nobars, subbars

mkReTrms	Make Random Effect Terms: Create Z, Lambda, Lind, etc.

# Description

From the result of findbars applied to a model formula and the evaluation frame fr, create the model matrix Zt, etc, associated with the random-effects terms.

## Usage

```
mkReTrms(bars, fr, drop.unused.levels=TRUE)
```

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## **Arguments**

bars a list of parsed random-effects terms

fr a model frame in which to evaluate these terms

drop.unused.levels

(logical) drop unused factor levels? (experimental)

## Value

## a list with components

Zt transpose of the sparse model matrix for the random effects

theta initial values of the covariance parameters

Lind an integer vector of indices determining the mapping of the elements of the

theta vector to the "x" slot of Lambdat

Gp a vector indexing the association of elements of the conditional mode vector

with random-effect terms; if nb is the vector of numbers of conditional modes per term (i.e. number of groups times number of effects per group), Gp is

c(0, cumsum(nb)) (and conversely nb is diff(Gp))

lower bounds on the covariance parameters

Lambdat transpose of the sparse relative covariance factor

flist list of grouping factors used in the random-effects terms

cnms a list of column names of the random effects according to the grouping factors

Ztlist list of components of the transpose of the random-effects model matrix, sepa-

rated by random-effects term

## See Also

Other utilities: findbars, mkRespMod, nlformula, nobars, subbars. getME can retrieve these components from a fitted model, although their values and/or forms may be slightly different in the final fitted model from their original values as returned from mkReTrms.

```
data("Pixel", package="nlme")
mform <- pixel ~ day + I(day^2) + (day | Dog) + (1 | Side/Dog)
(bar.f <- findbars(mform)) # list with 3 terms
mf <- model.frame(subbars(mform),data=Pixel)
rt <- mkReTrms(bar.f,mf)
names(rt)</pre>
```

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mkSimulateTemplate

Make templates suitable for guiding mixed model simulations

## **Description**

Make data and parameter templates suitable for guiding mixed model simulations, by specifying a model formula and other information (EXPERIMENTAL). Most useful for simulating balanced designs and for getting started on unbalanced simulations.

## Usage

```
mkParsTemplate(formula, data)
mkDataTemplate(formula, data, nGrps = 2, nPerGrp = 1, rfunc = NULL, ...)
```

## **Arguments**

formula A mixed model formula (see lmer).

data A data frame containing the names in formula.

nGrps Number of levels of a grouping factor. nPerGrp Number of observations per level.

rfunc Function for generating covariate data (e.g. rnorm.

... Additional parameters for rfunc.

## See Also

These functions are designed to be used with simulate.merMod.

mkVarCorr

Make Variance and Correlation Matrices from theta

## **Description**

Make variance and correlation matrices from theta

## Usage

```
mkVarCorr(sc, cnms, nc, theta, nms)
```

## **Arguments**

sc scale factor (residual standard deviation).

cnms component names.

nc numeric vector: number of terms in each RE component.

theta theta vector (lower-triangle of Cholesky factors).

nms component names (FIXME: nms/cnms redundant: nms=names(cnms)?)

#### Value

 $A\; {\tt matrix}$ 

#### See Also

VarCorr

modular

Modular Functions for Mixed Model Fits

## Description

Modular functions for mixed model fits

#### Usage

```
1Formula(formula, data = NULL, REML = TRUE, subset,
   weights, na.action, offset, contrasts = NULL,
   control = lmerControl(), ...)
mkLmerDevfun(fr, X, reTrms, REML = TRUE, start = NULL,
   verbose = 0, control = lmerControl(), ...)
optimizeLmer(devfun,
             optimizer
                          = formals(lmerControl)$optimizer,
             restart_edge = formals(lmerControl)$restart_edge,
             boundary.tol = formals(lmerControl)$boundary.tol,
             start = NULL, verbose = 0L,
             control = list(), ...)
glFormula(formula, data = NULL, family = gaussian,
    subset, weights, na.action, offset, contrasts = NULL,
   start, mustart, etastart, control = glmerControl(), ...)
mkGlmerDevfun(fr, X, reTrms, family, nAGQ = 1L,
              verbose = 0L, maxit = 100L, control = glmerControl(), ...)
optimizeGlmer(devfun, optimizer = "bobyqa",
   restart_edge = FALSE,
   boundary.tol = formals(glmerControl)$boundary.tol,
   verbose = 0L, control = list(),
   nAGQ = 1L, stage = 1, start = NULL, ...)
updateGlmerDevfun(devfun, reTrms, nAGQ = 1L)
```

## **Arguments**

formula a two-sided linear formula object describing both the fixed-effects and random-

effects parts of the model, with the response on the left of a ~ operator and the terms, separated by + operators, on the right. Random-effects terms are distinguished by vertical bars ("|") separating expressions for design matrices

from grouping factors.

data an optional data frame containing the variables named in formula. By default

the variables are taken from the environment from which lmer is called. While data is optional, the package authors *strongly* recommend its use, especially when later applying methods such as update and drop1 to the fitted model (*such methods are not guaranteed to work properly if* data *is omitted*). If data is omitted, variables will be taken from the environment of formula (if specified as a formula) or from the parent frame (if specified as a character vector).

REML (logical) indicating to fit **re**stricted maximum likelihood model.

subset an optional expression indicating the subset of the rows of data that should be

used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names

to be included. All observations are included by default.

weights an optional vector of 'prior weights' to be used in the fitting process. Should be

NULL or a numeric vector.

na.action a function that indicates what should happen when the data contain NAs. The de-

fault action (na.omit, inherited from the 'factory fresh' value of getOption("na.action"))

strips any observations with any missing values in any variables.

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.

contrasts an optional list. See the contrasts.arg of model.matrix.default.

control a list giving

**for** [g]lFormula: all options for running the model, see lmerControl;

 $\textbf{for} \ \mathsf{mkLmerDevfun}, \mathsf{mkGlmerDevfun} \textbf{:} \ \ \mathsf{options} \ \mathsf{for} \ \mathsf{the} \ \mathsf{inner} \ \mathsf{optimization} \ \mathsf{step};$ 

**for** optimizeLmer **and** optimizeGlmer: control parameters for nonlinear optimizer (typically inherited from the ... argument to lmerControl).

fr A model frame containing the variables needed to create an lmerResp or glmResp

instance.

X fixed-effects design matrix

reTrms information on random effects structure (see mkReTrms).

start starting values (see lmer; for glFormula, should be just a numeric vector of

fixed-effect coefficients)

verbose print output?

maxit maximal number of Pwrss update iterations.

devfun a deviance function, as generated by mkLmerDevfun

nAGQ

number of Gauss-Hermite quadrature points

stage

optimization stage (1: nAGQ=0, optimize over theta only; 2: nAGQ possibly >0, optimize over theta and beta)

optimizer

character - name of optimizing function(s). A character vector or list of functions: length 1 for 1mer or glmer, possibly length 2 for glmer. The built-in optimizers are "Nelder\_Mead" and "bobyqa" (from the minqa package). Any minimizing function that allows box constraints can be used provided that it

- 1. takes input parameters fn (function to be optimized), par (starting parameter values), lower (lower bounds) and control (control parameters, passed through from the control argument) and
- 2. returns a list with (at least) elements par (best-fit parameters), fval (best-fit function value), conv (convergence code) and (optionally) message (informational message, or explanation of convergence failure).

Special provisions are made for bobyqa, Nelder\_Mead, and optimizers wrapped in the optimx package; to use optimx optimizers (including L-BFGS-B from base optim and nlminb), pass the method argument to optim in the control argument.

For glmer, if length(optimizer)==2, the first element will be used for the preliminary (random effects parameters only) optimization, while the second will be used for the final (random effects plus fixed effect parameters) phase. See modular for more information on these two phases.

restart\_edge boundary.tol

see lmerControl see lmerControl

family

mustart

a GLM family; see glm and family.

etastart

optional starting values on the scale of the conditional mean; see glm for details. optional starting values on the scale of the unbounded predictor; see glm for

details.

other potential arguments; for optimizeLmer and optimizeGlmer, these are passed to internal function optwrap, which has relevant parameters calc. derivs and use.last.params (see lmerControl).

## **Details**

These functions make up the internal components of an [gn]lmer fit.

- [g]]Formula takes the arguments that would normally be passed to [g]]mer, checking for errors and processing the formula and data input to create a list of objects required to fit a mixed model.
- mk(Gl|L)merDevfun takes the output of the previous step (minus the formula component) and creates a deviance function
- optimize(G1|L)mer takes a deviance function and optimizes over theta (or over theta and beta, if stage is set to 2 for optimizeGlmer
- updateGlmerDevfun takes the first stage of a GLMM optimization (with nAGQ=0, optimizing over theta only) and produces a second-stage deviance function
- mkMerMod takes the *environment* of a deviance function, the results of an optimization, a list of random-effect terms, a model frame, and a model all and produces a [g]lmerMod object.

#### Value

1Formula and glFormula return a list containing components:

fr model frame

X fixed-effect design matrix

reTrms list containing information on random effects structure: result of mkReTrms

**REML** (lFormula only): logical indicating if restricted maximum likelihood was used (Copy of argument.)

mkLmerDevfun and mkGlmerDevfun return a function to calculate deviance (or restricted deviance) as a function of the theta (random-effect) parameters. updateGlmerDevfun returns a function to calculate the deviance as a function of a concatenation of theta and beta (fixed-effect) parameters. These deviance functions have an environment containing objects required for their evaluation. CAUTION: The environment of functions returned by mk(Gl|L)merDevfun contains reference class objects (see ReferenceClasses, merPredD-class, lmResp-class), which behave in ways that may surprise many users. For example, if the output of mk(Gl|L)merDevfun is naively copied, then modifications to the original will also appear in the copy (and vice versa). To avoid this behavior one must make a deep copy (see ReferenceClasses for details).

optimizeLmer and optimizeGlmer return the results of an optimization.

```
### Fitting a linear mixed model in 4 modularized steps
## 1. Parse the data and formula:
lmod <- lFormula(Reaction ~ Days + (Days|Subject), sleepstudy)</pre>
names(1mod)
## 2. Create the deviance function to be optimized:
(devfun <- do.call(mkLmerDevfun, lmod))</pre>
ls(environment(devfun)) # the environment of 'devfun' contains objects
                        # required for its evaluation
## 3. Optimize the deviance function:
opt <- optimizeLmer(devfun)</pre>
opt[1:3]
## 4. Package up the results:
mkMerMod(environment(devfun), opt, lmod$reTrms, fr = lmod$fr)
### Same model in one line
lmer(Reaction ~ Days + (Days|Subject), sleepstudy)
### Fitting a generalized linear mixed model in six modularized steps
## 1. Parse the data and formula:
glmod <- glFormula(cbind(incidence, size - incidence) ~ period + (1 | herd),</pre>
data = cbpp, family = binomial)
names(glmod)
## 2. Create the deviance function for optimizing over theta:
(devfun <- do.call(mkGlmerDevfun, glmod))</pre>
```

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NelderMead

Nelder-Mead Optimization of Parameters, Possibly (Box) Constrained

## **Description**

Nelder-Mead optimization of parameters, allowing optimization subject to box constraints (contrary to the default, method = "Nelder-Mead", in R's optim()), and using reverse communications.

## Usage

## **Arguments**

fn a function of a single numeric vector argument returning a numeric scalar.

par numeric vector of starting values for the parameters.

lower numeric vector of lower bounds (elements may be -Inf).

upper numeric vector of upper bounds (elements may be Inf).

control a named list of control settings. Possible settings are

**iprint** numeric scalar - frequency of printing evaluation information. Defaults to 0 indicating no printing.

**maxfun** numeric scalar - maximum number of function evaluations allowed (default:10000).

**FtolAbs** numeric scalar - absolute tolerance on change in function values (default: 1e-5)

**FtolRel** numeric scalar - relative tolerance on change in function values (default:1e-15)

**XtolRel** numeric scalar - relative tolerance on change in parameter values (default: 1e-7)

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**MinfMax** numeric scalar - maximum value of the minimum (default: .Machine\$double.xmin)

xst numeric vector of initial step sizes to establish the simplex - all elements must be non-zero (default: rep(0.02,length(par)))

xt numeric vector of tolerances on the parameters (default: xst\*5e-4)

**verbose** numeric value: 0=no printing, 1=print every 20 evaluations, 2=print every 10 evaluations, 3=print every evaluation. Sets 'iprint', if specified, but does not override it.

warnOnly a logical indicating if non-convergence (codes -1,-2,-3) should not stop(.), but rather only call warning and return a result which might inspected. Defaults to FALSE, i.e., stop on non-convergence.

### Value

a list with components

numeric scalar - the minimum function value achieved fval numeric vector - the value of x providing the minimum par integer valued scalar, if not 0, an error code: convergence -4 nm\_evals: maximum evaluations reached -3 nm\_forced: ? -2 nm\_nofeasible: cannot generate a feasible simplex -1 nm\_x0notfeasible: initial x is not feasible (?) 0 successful convergence message a string specifying the kind of convergence. the list of control settings after substituting for defaults. control feval the number of function evaluations.

### See Also

The NelderMead class definition and generator function.

NelderMead-class 71

```
o.2 <- Nelder_Mead(fr, p0, control=list(verbose=3, XtolRel=1e-15, FtolAbs= 1e-14)) all.equal(o.2[-5], o.1[-5], tolerance=1e-15)# TRUE, unexpectedly
```

NelderMead-class

Class "NelderMead" of Nelder-Mead optimizers and its Generator

## **Description**

Class "NelderMead" is a reference class for a Nelder-Mead simplex optimizer allowing box constraints on the parameters and using reverse communication.

The NelderMead() function conveniently generates such objects.

#### Usage

```
NelderMead(...)
```

## **Arguments**

... Argument list (see Note below).

#### Methods

```
NelderMead$new(lower, upper, xst, x0, xt)
Create a new NelderMead object
```

## Extends

All reference classes extend and inherit methods from "envRefClass".

#### Note

This is the default optimizer for the second stage of glmer and nlmer fits. We found that it was more reliable and often faster than more sophisticated optimizers.

Arguments to NelderMead() and the new method must be named arguments:

lower numeric vector of lower bounds - elements may be -Inf.

upper numeric vector of upper bounds - elements may be Inf.

xst numeric vector of initial step sizes to establish the simplex - all elements must be non-zero.

**x0** numeric vector of starting values for the parameters.

**xt** numeric vector of tolerances on the parameters.

## References

Based on code in the NLopt collection.

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## See Also

```
Nelder_Mead, the typical "constructor". Further, glmer, nlmer
```

## **Examples**

```
showClass("NelderMead")
```

ngrps

Number of Levels of a Factor or a "merMod" Model

## Description

Returns the number of levels of a factor or a set of factors, currently e.g., for each of the grouping factors of lmer(), glmer(), etc.

## Usage

```
ngrps(object, ...)
```

## **Arguments**

```
object an R object, see Details.
... currently ignored.
```

## **Details**

Currently there are methods for objects of class merMod, i.e., the result of lmer() etc, and factor objects.

#### Value

The number of levels (of a factor) or vector of number of levels for each "grouping factor" of a

```
ngrps(factor(seq(1,10,2)))
ngrps(lmer(Reaction ~ 1|Subject, sleepstudy))
## A named vector if there's more than one grouping factor :
ngrps(lmer(strength ~ (1|batch/cask), Pastes))
## cask:batch batch
## 30 10
methods(ngrps) # -> "factor" and "merMod"
```

nlformula 73

nlformula	Manipulate a Nonlinear Model Formula

### Description

Check and manipulate the formula for a nonlinear model, such as specified in nlmer.

# Usage

```
nlformula(mc)
```

### **Arguments**

mс

matched call from the calling function, typically nlmer(). Should have arguments named

**formula:** a formula of the form resp ~ nlmod ~ meform where resp is an expression for the response, nlmod is the nonlinear model expression and meform is the mixed-effects model formula. resp can be omitted when, e.g., optimizing a design.

data: a data frame in which to evaluate the model function

**start:** either a numeric vector containing initial estimates for the nonlinear model parameters or a list with components

nlpars: the initial estimates of the nonlinear model parameters theta: the initial estimates of the variance component parameters

### **Details**

The model formula for a nonlinear mixed-effects model is of the form resp ~ nlmod ~ mixed where resp is an expression (usually just a name) for the response, nlmod is the call to the nonlinear model function, and mixed is the mixed-effects formula defining the linear predictor for the parameter matrix. If the formula is to be used for optimizing designs, the resp part can be omitted.

# Value

a list with components

"respMod" a response module of class "nlsResp"

"frame" the model frame, including a terms attribute

"X" the fixed-effects model matrix

"reTrms" the random-effects terms object

### See Also

Other utilities: findbars, mkRespMod, mkReTrms, nobars, subbars

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nlmer

Fitting Nonlinear Mixed-Effects Models

### **Description**

Fit a nonlinear mixed-effects model (NLMM) to data, via maximum likelihood.

### Usage

```
nlmer(formula, data = NULL, control = nlmerControl(),
      start = NULL, verbose = 0L, nAGQ = 1L, subset, weights, na.action,
     offset, contrasts = NULL, devFunOnly = FALSE, ...)
```

# **Arguments**

formula

a three-part "nonlinear mixed model" formula, of the form resp ~ Nonlin(...) ~ fixed + random, where the third part is similar to the RHS formula of, e.g., lmer.

Currently, the Nonlin(...) formula part must not only return a numeric vector, but also must have a "gradient" attribute, a matrix. The functions SSbiexp, SSlogis, etc, see selfStart, provide this (and more). Alternatively, you can use deriv() to automatically produce such functions or expressions.

an optional data frame containing the variables named in formula. By default the variables are taken from the environment from which 1mer is called. While data is optional, the package authors strongly recommend its use, especially when later applying methods such as update and drop1 to the fitted model (such methods are not guaranteed to work properly if data is omitted). If data is omitted, variables will be taken from the environment of formula (if specified as a formula) or from the parent frame (if specified as a character vector).

a list (of correct class, resulting from lmerControl() or glmerControl() respectively) containing control parameters, including the nonlinear optimizer to be used and parameters to be passed through to the nonlinear optimizer, see the \*ImerControl documentation for details.

start

starting estimates for the nonlinear model parameters, as a named numeric vector or as a list with components

**nlpars** required numeric vector of starting values for the nonlinear model parameters

verbose

PIRLS steps.

**theta** optional numeric vector of starting values for the covariance parameters integer scalar. If > 0 verbose output is generated during the optimization of the parameter estimates. If > 1 verbose output is generated during the individual

nAGQ

integer scalar - the number of points per axis for evaluating the adaptive Gauss-Hermite approximation to the log-likelihood. Defaults to 1, corresponding to the Laplace approximation. Values greater than 1 produce greater accuracy in the evaluation of the log-likelihood at the expense of speed. A value of zero uses a faster but less exact form of parameter estimation for GLMMs by optimizing

data

control

nlmer 75

	the random effects and the fixed-effects coefficients in the penalized iteratively reweighted least squares step.
subset	an optional expression indicating the subset of the rows of data that should be used in the fit. This can be a logical vector, or a numeric vector indicating which observation numbers are to be included, or a character vector of the row names to be included. All observations are included by default.
weights	an optional vector of 'prior weights' to be used in the fitting process. Should be NULL or a numeric vector.
na.action	a function that indicates what should happen when the data contain NAs. The default action (na.omit, inherited from the 'factory fresh' value of getOption("na.action")) strips any observations with any missing values in any variables.
offset	this can be used to specify an <i>a priori</i> 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.
contrasts	an optional list. See the contrasts.arg of model.matrix.default.
devFunOnly	logical - return only the deviance evaluation function. Note that because the deviance function operates on variables stored in its environment, it may not return <i>exactly</i> the same values on subsequent calls (but the results should always be within machine tolerance).
	other potential arguments. A method argument was used in earlier versions of the package. Its functionality has been replaced by the nAGQ argument.

# **Details**

Fit nonlinear mixed-effects models, such as those used in population pharmacokinetics.

### Note

Adaptive Gauss-Hermite quadrature (nAGQ>1) is not currently implemented for nlmer. Several other methods, such as simulation or prediction with new data, are unimplemented or very lightly tested.

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```
## 3. Fit the same model with a user-built function:
## a. Define formula
nform <- ~Asym/(1+exp((xmid-input)/scal))</pre>
## b. Use deriv() to construct function:
nfun <- deriv(nform,namevec=c("Asym","xmid","scal"),</pre>
               function.arg=c("input","Asym","xmid","scal"))
nm1b <- update(nm1,circumference ~ nfun(age, Asym, xmid, scal) ~ Asym | Tree)
## 4. User-built function without using derivs():
      derivatives could be computed more efficiently
##
      by pre-computing components, but these are essentially
##
      the gradients as one would derive them by hand
nfun2 <- function(input, Asym, xmid, scal) {</pre>
    value <- Asym/(1+exp((xmid-input)/scal))</pre>
    grad <- cbind(Asym=1/(1+exp((xmid-input)/scal)),</pre>
              xmid=-Asym/(1+exp((xmid-input)/scal))^2*1/scal*
                     exp((xmid-input)/scal),
               scal=-Asym/(1+exp((xmid-input)/scal))^2*
                      -(xmid-input)/scal^2*exp((xmid-input)/scal))
    attr(value, "gradient") <- grad</pre>
    value
}
stopifnot(all.equal(attr(nfun(2,1,3,4),"gradient"),
                     attr(nfun(2,1,3,4), "gradient")))
nm1c <- update(nm1,circumference ~ nfun2(age, Asym, xmid, scal) ~ Asym | Tree)</pre>
```

nloptwrap

Wrappers for additional optimizers

### Description

Wrappers to allow use of alternative optimizers, from NLopt library or elsewhere, for nonlinear optimization stage

### **Usage**

```
nloptwrap(par, fn, lower, upper, control=list(),...)
nlminbwrap(par, fn, lower, upper, control=list(),...)
```

### **Arguments**

```
par starting parameter vector

fn objective function

lower vector of lower bounds

upper vector of upper bounds

control list of control parameters

... additional arguments to be passed to objective function
```

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### **Details**

Using alternative optimizers is an important trouble-shooting tool for mixed models. These wrappers provide convenient access to the optimizers provided by Steven Johnson's NLopt library (via the nloptr R package), and to the nlminb optimizer from base R. (nlminb is also available via the optimx package; this wrapper provides access to nlminb without the need to install/link the package, and without the additional post-fitting checks that are implemented by optimx (see examples below).

One important difference between the nloptr-provided implementation of BOBYQA and the minqa-provided version accessible via optimizer="bobyqa" is that it provides simpler access to optimization tolerances. minqa::bobyqa provides only the rhoend parameter ("[t]he smallest value of the trust region radius that is allowed"), while nloptr provides a more standard set of tolerances for relative or absolute change in the objective function or the parameter values (ftol\_rel, ftol\_abs, xtol\_rel, xtol\_abs).

### Value

par estimated parameters

fval objective function value at minimum

feval number of function evaluations

conv convergence code (0 if no error)

message convergence message

### Author(s)

Gabor Grothendieck (nlminbwrap)

78 Pastes

nobars

Omit terms separated by vertical bars in a formula

### **Description**

Remove the random-effects terms from a mixed-effects formula, thereby producing the fixed-effects formula.

# Usage

```
nobars(term)
```

# Arguments

term

the right-hand side of a mixed-model formula

### Value

the fixed-effects part of the formula

### Note

This function is called recursively on individual terms in the model, which is why the argument is called term and not a name like form, indicating a formula.

### See Also

```
formula, model.frame, model.matrix.
Other utilities: findbars, mkRespMod, mkReTrms, nlformula, subbars
```

### **Examples**

```
nobars(Reaction ~ Days + (Days|Subject)) ## => Reaction ~ Days
```

**Pastes** 

Paste strength by batch and cask

# **Description**

Strength of a chemical paste product; its quality depending on the delivery batch, and the cask within the delivery.

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### **Format**

A data frame with 60 observations on the following 4 variables.

```
strength paste strength.
```

batch delivery batch from which the sample was sample. A factor with 10 levels: 'A' to 'J'.

cask cask within the delivery batch from which the sample was chosen. A factor with 3 levels: 'a' to 'c'.

sample the sample of paste whose strength was assayed, two assays per sample. A factor with 30 levels: 'A:a' to 'J:c'.

#### **Details**

The data are described in Davies and Goldsmith (1972) as coming from "deliveries of a chemical paste product contained in casks where, in addition to sampling and testing errors, there are variations in quality between deliveries ... As a routine, three casks selected at random from each delivery were sampled and the samples were kept for reference. ... Ten of the delivery batches were sampled at random and two analytical tests carried out on each of the 30 samples".

#### Source

O.L. Davies and P.L. Goldsmith (eds), *Statistical Methods in Research and Production*, 4th ed., Oliver and Boyd, (1972), section 6.5

```
str(Pastes)
require(lattice)
dotplot(cask ~ strength | reorder(batch, strength), Pastes,
        strip = FALSE, strip.left = TRUE, layout = c(1, 10),
        ylab = "Cask within batch",
        xlab = "Paste strength", jitter.y = TRUE)
## Modifying the factors to enhance the plot
Pastes <- within(Pastes, batch <- reorder(batch, strength))</pre>
Pastes <- within(Pastes, sample <- reorder(reorder(sample, strength),
          as.numeric(batch)))
dotplot(sample ~ strength | batch, Pastes,
        strip = FALSE, strip.left = TRUE, layout = c(1, 10),
        scales = list(y = list(relation = "free")),
        ylab = "Sample within batch",
        xlab = "Paste strength", jitter.y = TRUE)
## Four equivalent models differing only in specification
(fm1 <- lmer(strength ~ (1|batch) + (1|sample), Pastes))</pre>
(fm2 <- lmer(strength ~ (1|batch/cask), Pastes))</pre>
(fm3 <- lmer(strength ~ (1|batch) + (1|batch:cask), Pastes))</pre>
(fm4 <- lmer(strength ~ (1|batch/sample), Pastes))</pre>
## fm4 results in redundant labels on the sample:batch interaction
head(ranef(fm4)[[1]])
## compare to fm1
head(ranef(fm1)[[1]])
## This model is different and NOT appropriate for these data
```

80 Penicillin

```
(fm5 <- lmer(strength ~ (1|batch) + (1|cask), Pastes))
L <- getME(fm1, "L")
Matrix::image(L, sub = "Structure of random effects interaction in pastes model")</pre>
```

Penicillin

Variation in penicillin testing

### **Description**

Six samples of penicillin were tested using the *B. subtilis* plate method on each of 24 plates. The response is the diameter (mm) of the zone of inhibition of growth of the organism.

### **Format**

A data frame with 144 observations on the following 3 variables.

```
diameter diameter (mm) of the zone of inhibition of the growth of the organism. plate assay plate. A factor with levels 'a' to 'x'. sample penicillin sample. A factor with levels 'A' to 'F'.
```

#### **Details**

The data are described in Davies and Goldsmith (1972) as coming from an investigation to "assess the variability between samples of penicillin by the *B. subtilis* method. In this test method a bulk-inoculated nutrient agar medium is poured into a Petri dish of approximately 90 mm. diameter, known as a plate. When the medium has set, six small hollow cylinders or pots (about 4 mm. in diameter) are cemented onto the surface at equally spaced intervals. A few drops of the penicillin solutions to be compared are placed in the respective cylinders, and the whole plate is placed in an incubator for a given time. Penicillin diffuses from the pots into the agar, and this produces a clear circular zone of inhibition of growth of the organisms, which can be readily measured. The diameter of the zone is related in a known way to the concentration of penicillin in the solution."

# Source

O.L. Davies and P.L. Goldsmith (eds), *Statistical Methods in Research and Production*, 4th ed., Oliver and Boyd, (1972), section 6.6

plot.merMod 81

plot.merMod

Diagnostic Plots for 'merMod' Fits

### **Description**

diagnostic plots for merMod fits

### Usage

```
## S3 method for class 'merMod'
plot(x,
    form = resid(., type = "pearson") ~ fitted(.), abline,
    id = NULL, idLabels = NULL, grid, ...)
## S3 method for class 'merMod'
qqmath(x, id = NULL, idLabels = NULL, ...)
```

#### **Arguments**

x a fitted [ng]lmer model

form

an optional formula specifying the desired type of plot. Any variable present in the original data frame used to obtain x can be referenced. In addition, x itself can be referenced in the formula using the symbol ".". Conditional expressions on the right of a | operator can be used to define separate panels in a lattice display. Default is resid(., type = "pearson") ~ fitted(.), corresponding to a plot of the standardized residuals versus fitted values.

abline

an optional numeric value, or numeric vector of length two. If given as a single value, a horizontal line will be added to the plot at that coordinate; else, if given as a vector, its values are used as the intercept and slope for a line added to the plot. If missing, no lines are added to the plot.

id

an optional numeric value, or one-sided formula. If given as a value, it is used as a significance level for a two-sided outlier test for the standardized, or normalized residuals. Observations with absolute standardized (normalized) residuals greater than the 1-value/2 quantile of the standard normal distribution are identified in the plot using idLabels. If given as a one-sided formula, its right hand side must evaluate to a logical, integer, or character vector which is used to identify observations in the plot. If missing, no observations are identified.

idLabels

an optional vector, or one-sided formula. If given as a vector, it is converted to character and used to label the observations identified according to id. If given as a vector, it is converted to character and used to label the observations identified according to id. If given as a one-sided formula, its right hand side must evaluate to a vector which is converted to character and used to label the identified observations. Default is the interaction of all the grouping variables in the data frame. The special formula idLabels=~. obs will label the observations according to observation number.

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an optional logical value indicating whether a grid should be added to plot. Default depends on the type of lattice plot used: if xyplot defaults to TRUE, else defaults to FALSE.

... optional arguments passed to the lattice plot function.

### **Details**

Diagnostic plots for the linear mixed-effects fit are obtained. The form argument gives considerable flexibility in the type of plot specification. A conditioning expression (on the right side of a | operator) always implies that different panels are used for each level of the conditioning factor, according to a lattice display. If form is a one-sided formula, histograms of the variable on the right hand side of the formula, before a | operator, are displayed (the lattice function histogram is used). If form is two-sided and both its left and right hand side variables are numeric, scatter plots are displayed (the lattice function xyplot is used). Finally, if form is two-sided and its left had side variable is a factor, box-plots of the right hand side variable by the levels of the left hand side variable are displayed (the lattice function bwplot is used).

qqmath produces a Q-Q plot of the residuals (see qqmath.ranef.mer for Q-Q plots of the conditional mode values).

### Author(s)

original version in n1me package by Jose Pinheiro and Douglas Bates

```
data(Orthodont,package="nlme")
fm1 <- lmer(distance ~ age + (age|Subject), data=Orthodont)</pre>
## standardized residuals versus fitted values by gender
plot(fm1, resid(., scaled=TRUE) ~ fitted(.) | Sex, abline = 0)
## box-plots of residuals by Subject
plot(fm1, Subject ~ resid(., scaled=TRUE))
## observed versus fitted values by Subject
plot(fm1, distance \sim fitted(.) \mid Subject, abline = c(0,1))
## residuals by age, separated by Subject
plot(fm1, resid(., scaled=TRUE) ~ age | Sex, abline = 0)
require("lattice")
qqmath(fm1, id=0.05)
if (require("ggplot2")) {
    ## we can create the same plots using ggplot2 and the fortify() function
    fm1F <- fortify.merMod(fm1)</pre>
    ggplot(fm1F, aes(.fitted,.resid)) + geom_point(colour="blue") +
           facet_grid(.~Sex) + geom_hline(yintercept=0)
    ## note: Subjects are ordered by mean distance
    ggplot(fm1F, aes(Subject,.resid)) + geom_boxplot() + coord_flip()
    ggplot(fm1F, aes(.fitted,distance))+ geom_point(colour="blue") +
        facet_wrap(~Subject) +geom_abline(intercept=0,slope=1)
    ggplot(fm1F, aes(age,.resid)) + geom_point(colour="blue") + facet_grid(.~Sex) +
      geom_hline(yintercept=0)+geom_line(aes(group=Subject),alpha=0.4)+geom_smooth(method="loess")
    ## (warnings about loess are due to having only 4 unique x values)
    detach("package:ggplot2")
}
```

plots.thpr 83

plots.thpr

Mixed-Effects Profile Plots (Regular / Density / Pairs)

# Description

Xyplot, Densityplot, and Pairs plot methods for a mixed-effects model profile.

xyplot() draws "zeta diagrams", also visualizing confidence intervals and their asymmetry.

densityplot() draws the profile densities.

splom() draws profile pairs plots. Contours are for the marginal two-dimensional regions (i.e. using df = 2).

# Usage

### **Arguments**

х	a mixed-effects profile, i.e., of class "thpr", typically resulting from profile(fm) where fm is a fitted model from lmer (or its generalizations).
data	unused - only for compatibility with generic.
levels	the contour levels to be shown; usually derived from conf.
conf	numeric vector of confidence levels to be shown as contours.
absVal	logical indicating if abs(.)olute values should be plotted, often preferred for confidence interval visualization.
scales	plotting options to be passed to xyplot
which	integer or character vector indicating which parameters to profile: default is all parameters (see profile-methods for details).
draw.lower	(logical) draw lower-triangle (zeta scale) panels?
draw.upper	(logical) draw upper-triangle (standard dev/cor scale) panels?
	further arguments passed to xyplot, densityplot, or splom from package <b>lattice</b> , respectively.

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### Value

xyplot: a density plot, a "trellis" object (lattice package) which when print()ed produces plots on the current graphic device.

**densityplot:** a density plot, a "trellis" object, see above.

splom: a pairs plot, aka scatterplot matrix, a "trellis" object, see above.

#### See Also

```
profile, notably for an example.
```

# Examples

```
## see example("profile.merMod")
```

predict.merMod

Predictions from a model at new data values

### **Description**

The predict method for merMod objects, i.e. results of lmer(), glmer(), etc.

# Usage

# **Arguments**

object a fitted model object

newdata data frame for which to evaluate predictions.

newparams new parameters to use in evaluating predictions, specified as in the start pa-

rameter for lmer or glmer – a list with components theta and/or (for GLMMs)

beta.

re.form formula for random effects to condition on. If NULL, include all random effects;

if NA or ~0, include no random effects.

Reform, REform, REform

allowed for backward compatibility: re.form is now the preferred argument

name.

random.only (logical) ignore fixed effects, making predictions only using random effects?

terms a terms object - unused at present.

type character string - either "link", the default, or "response" indicating the type of prediction object returned.

allow.new.levels
logical if new levels (or NA values) in newdata are allowed. If FALSE (default), such new values in newdata will trigger an error; if TRUE, then the prediction will use the unconditional (population-level) values for data with previously unobserved levels (or NAs).

na.action
function determining what should be done with missing values for fixed effects in newdata. The default is to predict NA: see na.pass.

optional additional parameters. None are used at present.

### **Details**

- If any random effects are included in re.form (see below), newdata *must* contain columns corresponding to all of the grouping variables and random effects used in the original model, even if not all are used in prediction; however, they can be safely set to NA in this case.
- There is no option for computing standard errors of predictions because it is difficult to define
  an efficient method that incorporates uncertainty in the variance parameters; we recommend
  bootMer for this task.

#### Value

a numeric vector of predicted values

# **Examples**

```
(gm1 <- glmer(cbind(incidence, size - incidence) ~ period + (1 |herd), cbpp, binomial))
str(p0 <- predict(gm1))  # fitted values
str(p1 <- predict(gm1,re.form=NA)) # fitted values, unconditional (level-0)
newdata <- with(cbpp, expand.grid(period=unique(period), herd=unique(herd)))
str(p2 <- predict(gm1,newdata)) # new data, all RE
str(p3 <- predict(gm1,newdata,re.form=NA)) # new data, level-0
str(p4 <- predict(gm1,newdata,re.form= ~(1|herd))) # explicitly specify RE
stopifnot(identical(p2, p4))</pre>
```

profile-methods

Profile method for merMod objects

### **Description**

Methods for profile() of [ng]lmer fitted models.

The log() method and the more flexible logProf() utility transform a lmer profile into one where logarithms of standard deviations are used, while varianceProf converts from the standard-deviation to the variance scale; see Details.

### Usage

```
## S3 method for class 'merMod'
profile(fitted, which = NULL, alphamax = 0.01,
maxpts = 100, delta = NULL,
        delta.cutoff = 1/8, verbose = 0, devtol = 1e-09,
        maxmult = 10, startmethod = "prev", optimizer = NULL,
        control=NULL, signames = TRUE,
        parallel = c("no", "multicore", "snow"),
        ncpus = getOption("profile.ncpus", 1L), cl = NULL,
        prof.scale = c("sdcor", "varcov"),
## S3 method for class 'thpr'
as.data.frame(x, ...)
## S3 method for class 'thpr'
log(x, base = exp(1))
logProf(x, base = exp(1), ranef = TRUE,
           sigIni = if(ranef) "sig" else "sigma")
varianceProf(x, ranef = TRUE)
```

# **Arguments**

fitted

a fitted model, e.g., the result of lmer(..).

which

NULL value, integer or character vector indicating which parameters to profile: default (NULL) is all parameters. For integer, i.e., indexing, the parameters are ordered as follows:

- (1) random effects (theta) parameters; these are ordered as in getME(., "theta"), i.e., as the lower triangle of a matrix with standard deviations on the diagonal and correlations off the diagonal.
- (2) residual standard deviation (or scale parameter for GLMMs where appropriate).
- (3) fixed effect (beta) parameters.

Alternatively, which may be a character, containing "beta\_" or "theta\_" denoting the fixed or random effects parameters, respectively, or also containing parameter names, such as ".sigma" or "(Intercept)".

alphamax

a number in (0,1), such that 1 - alphamax is the maximum alpha value for likelihood ratio confidence regions; used to establish the range of values to be profiled.

maxpts

maximum number of points (in each direction, for each parameter) to evaluate in attempting to construct the profile.

delta

stepping scale for deciding on next point to profile. The code uses the local derivative of the profile at the current step to establish a change in the focal parameter that will lead to a step of delta on the square-root-deviance scale. If NULL, the delta.cutoff parameter will be used to determine the stepping scale.

delta.cutoff

stepping scale (see delta) expressed as a fraction of the target maximum value of the profile on the square-root-deviance scale. Thus a delta.cutoff setting of 1/n will lead to a profile with approximately 2\*n calculated points for each

. 1 .. |. . ... . . .

	parameter (i.e., n points in each direction, below and above the estimate for each parameter).
verbose	level of output from internal calculations.
devtol	tolerance for fitted deviances less than baseline (supposedly minimum) deviance.
maxmult	maximum multiplier of the original step size allowed, defaults to 10.
startmethod	method for picking starting conditions for optimization (STUB).
optimizer	(character or function) optimizer to use (see lmer for details); default is to use the optimizer from the original model fit.
control	a list of options controlling the profiling (see lmerControl): default is to use the control settings from the original model fit.
signames	logical indicating if abbreviated names of the form .sigNN should be used; otherwise, names are more meaningful (but longer) of the form (sd cor)_(effects) (group). Note that some code for profile transformations (e.g., log() or varianceProf) depends on signames==TRUE.
	potential further arguments for various methods.
X	an object of class thpr (i.e., output of profile)
base	the base of the logarithm. Defaults to natural logarithms.
ranef	logical indicating if the sigmas of the random effects should be $log()$ transformed as well. If false, only $\sigma$ (standard deviation of errors) is transformed.
sigIni	character string specifying the initial part of the sigma parameters to be log transformed.
parallel	The type of parallel operation to be used (if any). If missing, the default is taken from the option "profile.parallel" (and if that is not set, "no").
ncpus	integer: number of processes to be used in parallel operation: typically one would choose this to be the number of available CPUs.
cl	An optional <b>parallel</b> or <b>snow</b> cluster for use if parallel = "snow". If not supplied, a cluster on the local machine is created for the duration of the profile call.
prof.scale	whether to profile on the standard deviation-correlation scale ("sdcor") or on the variance-covariance scale ("varcov")

# **Details**

The log method and the more flexible logProf() function transform the profile into one where  $\log(\sigma)$  is used instead of  $\sigma$ . By default all sigmas including the standard deviations of the random effects are transformed i.e., the methods return a profile with all of the .sigNN parameters replaced by .lsigNN. If ranef is false, only ".sigma", the standard deviation of the errors, is transformed (as it should never be zero, whereas random effect standard deviations (.sigNN) can be reasonably be zero).

The forward and backward splines for the log-transformed parameters are recalculated. Note that correlation parameters are not handled sensibly at present (i.e., they are logged rather than taking a more applicable transformation such as an arc-hyperbolic tangent,  $\operatorname{atanh}(x) = \log((1+x)/(1-x))/2$ ).

The varianceProf function works similarly, including non-sensibility for correlation parameters, by squaring all parameter values, changing the names by appending sq appropriately (e.g. .sigNN to .sigsqNN). Setting prof.scale="varcov" in the original profile() call is a more computationally intensive, but more correct, way to compute confidence intervals for covariance parameters.

Methods for function profile (package stats), here for profiling (fitted) mixed effect models.

### Value

profile(<merMod>) returns an object of S3 class "thpr", which is data.frame-like. Notable methods for such a profile object confint(), which returns the confidence intervals based on the profile, and three plotting methods (which require the lattice package), xyplot, densityplot, and splom.

In addition, the log() (see above) and as.data.frame() methods can transform "thpr" objects in useful ways.

### See Also

The plotting methods xyplot etc, for class "thpr".

For (more expensive) alternative confidence intervals: bootMer.

```
fm01ML <- lmer(Yield ~ 1|Batch, Dyestuff, REML = FALSE)</pre>
system.time(
 tpr <- profile(fm01ML, optimizer="Nelder_Mead", which="beta_")</pre>
)## fast; as only *one* beta parameter is profiled over
## full profiling (default which means 'all) needs
## ~2.6s (on a 2010 Macbook Pro)
system.time( tpr <- profile(fm01ML))</pre>
## ~1s, + possible warning about bobyqa convergence
(confint(tpr) -> CIpr)
stopifnot(all.equal(unname(CIpr),
 array(c(12.1985292, 38.2299848, 1486.4515,
          84.0630513, 67.6576964, 1568.54849), dim = 3:2),
                    tol= 1e-07))# 1.37e-9 {64b}
library("lattice")
xyplot(tpr)
xyplot(tpr, absVal=TRUE) # easier to see conf.int.s (and check symmetry)
xyplot(tpr, conf = c(0.95, 0.99), # (instead of all five 50, 80,...)
       main = "95% and 99% profile() intervals")
xyplot(logProf(tpr, ranef=FALSE),
       main = expression("lmer profile()s"~~ log(sigma)*" (only log)"))
densityplot(tpr, main="densityplot( profile(lmer(..)) )")
densityplot(varianceProf(tpr), main=" varianceProf( profile(lmer(..)) )")
splom(tpr)
splom(logProf(tpr, ranef=FALSE))
doMore <- lme4:::testLevel() > 1
if(doMore) { ## not typically, for time constraint reasons
## Batch and residual variance only
```

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```
system.time(tpr2 <- profile(fm01ML, which=1:2, optimizer="Nelder_Mead"))</pre>
print( xyplot(tpr2) )
print( xyplot(log(tpr2)) )# log(sigma) is better
print( xyplot(logProf(tpr2, ranef=FALSE)) )
## GLMM example
gm1 <- glmer(cbind(incidence, size - incidence) ~ period + (1 | herd),</pre>
     data = cbpp, family = binomial)
## running ~ 10-12 seconds on a modern machine {-> "verbose" while you wait}:
print( system.time(pr4 <- profile(gm1, verbose=TRUE)) )</pre>
print( xyplot(pr4, layout=c(5,1), as.table=TRUE) )
print( xyplot(log(pr4), absVal=TRUE) ) # log(sigma_1)
print( splom(pr4) )
print( system.time( # quicker: only sig01 and one fixed effect
     pr2 <- profile(gm1, which=c("theta_", "period2"))))</pre>
print( confint(pr2) )
## delta..: higher underlying resolution, only for 'sigma_1':
print( system.time(
     pr4.hr <- profile(gm1, which="theta_", delta.cutoff=1/16)))</pre>
print( xyplot(pr4.hr) )
}
```

prt-utilities

Print and Summary Method Utilities for Mixed Effects

# Description

The print, summary methods (including the print for the summary() result) in **lme4** are modular, using about ten small utility functions. Other packages, building on **lme4** can use the same utilities for ease of programming and consistency of output.

Notably see the Examples.

11ikAIC() extracts the log likelihood, AIC, and related statics from a Fitted LMM.

formatVC() "format()"s the VarCorr matrix of the random effects – for print()ing and show()ing; it is also the "workhorse" of .prt.VC(), and returns a character matrix.

.prt.\*() all use cat and print to produce output.

### Usage

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### **Arguments**

object a LMM model fit

devianceFUN the function to be used for computing the deviance; should not be changed for

**lme4** created objects.

chkREML optional logical indicating if object maybe a REML fit.

devcomp for **lme4** always the equivalent of object@devcomp; here a list

dims for **lme4** always the equivalent of object@devcomp\$dims, a named vector or

list with components "GLMM", "NLMM", "REML", and "nAGQ" of which the first two are logical scalars, and the latter two typically are FALSE or numeric.

mtit the result of methTitle(object)

class typically class(object).

famL a list with components family and link, each a character string; note that

standard R family objects can be used directly, as well.

resids numeric vector of model residuals.

digits non-negative integer of (significant) digits to print minimally.

title character string.

... optional arguments passed on, e.g., to residuals().

the call of the model fit; e.g., available via (generic) function getCall().

long logical indicating if the output may be long, e.g., printing the control part of

the call if there is one.

aictab typically the AICtab component of the result of llikAIC().

varcor typically the result of VarCorr().

comp optional ...

formatter a function used for formatting the numbers.

ngrps integer (vector), typically the result of ngrps(object).

nobs integer; the number of observations, e.g., the result of nobs.

optinfo typically object @ optinfo, the optimization infos, including warnings if there

were.

summary logical

useScale (logical) whether the parent model estimates a scale parameter

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### Value

```
llikAIC() returns a list with components

logLik which is logLik(object), and

AICtab a "table" of AIC, BIC, logLik, deviance and df.residual() values.
```

```
## Create a few "lme4 standard" models ------
fm1 <- lmer(Reaction ~ Days + (Days | Subject), sleepstudy)</pre>
fmM <- update(fm1, REML=FALSE) # -> Maximum Likelihood
gm1 <- glmer(cbind(incidence, size - incidence) ~ period + (1 | herd),</pre>
             data = cbpp, family = binomial)
gmA \leftarrow update(gm1, nAGQ = 5)
(lA1 <- llikAIC(fm1))</pre>
(lam <- llikaIC(fmM))</pre>
(lAg <- llikAIC(gmA))</pre>
(m1 <- methTitle(fm1 @ devcomp $ dims))</pre>
(mM <- methTitle(fmM @ devcomp $ dims))</pre>
(mG <- methTitle(gm1 @ devcomp $ dims))</pre>
(mA <- methTitle(gmA @ devcomp $ dims))</pre>
.prt.methTit(m1, class(fm1))
.prt.methTit(mA, class(gmA))
.prt.family(gaussian())
.prt.family(binomial())
.prt.family( poisson())
.prt.resids(residuals(fm1), digits = 4)
.prt.resids(residuals(fmM), digits = 2)
.prt.call(getCall(fm1))
.prt.call(getCall(gm1))
.prt.aictab ( lA1 $ AICtab ) # REML
.prt.aictab ( lAM $ AICtab ) # ML --> AIC, BIC, ...
V1 <- VarCorr(fm1)
m <- formatVC(V1)</pre>
stopifnot(is.matrix(m), is.character(m), ncol(m) == 4)
print(m, quote = FALSE) ## prints all but the first line of .prt.VC() below:
.prt.VC( V1, digits = 4, formatter = format)
## Random effects:
## Groups Name
                         Std.Dev. Corr
## Subject (Intercept) 24.740
                         5.922
##
             Days
                                  0.07
                         25.592
## Residual
```

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pvalues

Getting p-values for fitted models

### **Description**

One of the most frequently asked questions about 1me4 is "how do I calculate p-values for estimated parameters?" Previous versions of 1me4 provided the mcmcsamp function, which efficiently generated a Markov chain Monte Carlo sample from the posterior distribution of the parameters, assuming flat (scaled likelihood) priors. Due to difficulty in constructing a version of mcmcsamp that was reliable even in cases where the estimated random effect variances were near zero (e.g. https://stat.ethz.ch/pipermail/r-sig-mixed-models/2009q4/003115.html), mcmcsamp has been withdrawn (or more precisely, not updated to work with 1me4 versions >=1.0.0).

Many users, including users of the aovlmer.fnc function from the languageR package which relies on mcmcsamp, will be deeply disappointed by this lacuna. Users who need p-values have a variety of options. In the list below, the methods marked MC provide explicit model comparisons; CI denotes confidence intervals; and P denotes parameter-level or sequential tests of all effects in a model. The starred (\*) suggestions provide finite-size corrections (important when the number of groups is <50); those marked (+) support GLMMs as well as LMMs.

- likelihood ratio tests via anova or drop1 (MC,+)
- profile confidence intervals via profile.merMod and confint.merMod (CI,+)
- parametric bootstrap confidence intervals and model comparisons via bootMer (or PBmodcomp in the pbkrtest package) (MC/CI,\*,+)
- for random effects, simulation tests via the RLRsim package (MC,\*)
- for fixed effects, F tests via Kenward-Roger approximation using KRmodcomp from the pbkrtest package (MC,\*)
- car::Anova and lmerTest::anova provide wrappers for Kenward-Roger-corrected tests using pbkrtest: lmerTest::anova also provides t tests via the Satterthwaite approximation (P,\*)
- afex::mixed is another wrapper for pbkrtest and anova providing "Type 3" tests of all effects (P,\*,+)

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arm::sim, or bootMer, can be used to compute confidence intervals on predictions.

For glmer models, the summary output provides p-values based on asymptotic Wald tests (P); while this is standard practice for generalized linear models, these tests make assumptions both about the shape of the log-likelihood surface and about the accuracy of a chi-squared approximation to differences in log-likelihoods.

When all else fails, don't forget to keep p-values in perspective: http://www.phdcomics.com/comics/archive.php?comicid=905

ranef

Extract the modes of the random effects

# Description

A generic function to extract the conditional modes of the random effects from a fitted model object. For linear mixed models the conditional modes of the random effects are also the conditional means.

# Usage

# Arguments

object	an object of a class of fitted models with random effects, typically a merMod object.
condVar	an optional logical argument indicating if the conditional variance-covariance matrices of the random effects should be added as an attribute.
drop	should components of the return value that would be data frames with a single column, usually a column called '(Intercept)', be returned as named vectors instead?
whichel	character vector of names of grouping factors for which the random effects should be returned.
postVar	a (deprecated) synonym for condVar
X	a random-effects object (of class ranef.mer) produced by ranef
main	include a main title, indicating the grouping factor, on each sub-plot?
transf	transformation for random effects: for example, exp for plotting parameters from a (generalized) logistic regression on the odds rather than log-odds scale
data	This argument is required by the dotplot and qqmath generic methods, but is not actually used.
	some methods for these generic functions require additional arguments.

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### **Details**

If grouping factor i has k levels and j random effects per level the ith component of the list returned by ranef is a data frame with k rows and j columns. If condVar is TRUE the "postVar" attribute is an array of dimension j by j by k. The kth face of this array is a positive definite symmetric j by j matrix. If there is only one grouping factor in the model the variance-covariance matrix for the entire random effects vector, conditional on the estimates of the model parameters and on the data will be block diagonal and this j by j matrix is the kth diagonal block. With multiple grouping factors the faces of the "postVar" attributes are still the diagonal blocks of this conditional variance-covariance matrix but the matrix itself is no longer block diagonal.

#### Value

An object of class ranef.mer composed of a list of data frames, one for each grouping factor for the random effects. The number of rows in the data frame is the number of levels of the grouping factor. The number of columns is the dimension of the random effect associated with each level of the factor.

If condVar is TRUE each of the data frames has an attribute called "postVar" which is a threedimensional array with symmetric faces; each face contains the variance-covariance matrix for a particular level of the grouping factor. (The name of this attribute is a historical artifact, and may be changed to condVar at some point in the future.)

When drop is TRUE any components that would be data frames of a single column are converted to named numeric vectors.

#### Note

To produce a (list of) "caterpillar plots" of the random effects apply dotplot to the result of a call to ranef with condVar = TRUE; qqmath will generate a list of Q-Q plots.

```
require(lattice)
fm1 <- lmer(Reaction ~ Days + (Days|Subject), sleepstudy)</pre>
fm2 <- lmer(Reaction ~ Days + (1|Subject) + (0+Days|Subject), sleepstudy)</pre>
fm3 <- lmer(diameter ~ (1|plate) + (1|sample), Penicillin)
ranef(fm1)
str(rr1 <- ranef(fm1, condVar = TRUE))</pre>
dotplot(rr1) ## default
## specify free scales in order to make Day effects more visible
dotplot(rr1,scales = list(x = list(relation = 'free')))[["Subject"]]
if(FALSE) { ##-- condVar=TRUE is not yet implemented for multiple terms -- FIXME
    str(ranef(fm2, condVar = TRUE))
}
op <- options(digits = 4)
ranef(fm3, drop = TRUE)
options(op)
## extracting random effects and conditional standard deviations
dd <- as.data.frame(rr1)</pre>
if (require(ggplot2)) {
   ggplot(dd,aes(y=grp,x=condval))+
        geom_point()+facet_wrap(~term, scales="free_x")+
```

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```
\label{eq:geom_error} geom\_errorbarh(aes(xmin=condval-2*condsd,xmax=condval+2*condsd),\\ height=0) }
```

refit

Refit a (merMod) Model with a Different Response

# **Description**

Refit a model, possibly after modifying the response vector. This makes use of the model representation and directly goes to the optimization.

### Usage

# **Arguments**

object a fitted model, usually of class lmerMod, to be refit with a new response.

newresp an (optional) numeric vector providing the new response, of the same length as

the original response (see Details for information on NA handling). May also

be a data frame with a single numeric column, e.g. as produced by simulate(object).

rename.response

when refitting the model, should the name of the response variable in the formula

and model frame be replaced with the name of newresp?

maxit scalar integer, currently only for GLMMs: the maximal number of Pwrss update

iterations.

... optional additional parameters. For the merMod method, control.

### **Details**

Refit a model, possibly after modifying the response vector. This could be done using update(), but the refit() approach should be faster because it bypasses the creation of the model representation and goes directly to the optimization step.

Setting rename.response = TRUE may be necessary if one wants to do further operations (such as update) on the fitted model. However, the refitted model will still be slightly different from the equivalent model fitted via update; in particular, the terms component is not updated to reflect the new response variable, if it has a different name from the original.

If newresp has an na.action attribute, then it is assumed that NA values have already been removed from the numeric vector; this allows the results of simulate(object) to be used even if the original response vector contained NA values. Otherwise, the length of newresp must be the same as the *original* length of the response.

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### Value

an object like x, but fit to a different response vector Y.

#### See Also

update.merMod for more flexible and extensive model refitting; refitML for refitting a REML fitted model with maximum likelihood ('ML').

### **Examples**

```
## Ex. 1: using refit() to fit each column in a matrix of responses ------
set.seed(101)
Y <- matrix(rnorm(1000),ncol=10)
## combine first column of responses with predictor variables
d <- data.frame(y=Y[,1],x=rnorm(100),f=rep(1:10,10))</pre>
## (use check.conv.grad="ignore" to disable convergence checks because we
## are using a fake example)
## fit first response
fit1 <- lmer(y \sim x+(1|f), data = d,
             control= lmerControl(check.conv.grad="ignore",
                                   check.conv.hess="ignore"))
## combine fit to first response with fits to remaining responses
res <- c(fit1,lapply(as.data.frame(Y[,-1]), refit, object=fit1))</pre>
## Ex. 2: refitting simulated data using data that contain NA values -----
sleepstudyNA <- sleepstudy
sleepstudyNA$Reaction[1:3] <- NA</pre>
fm0 <- lmer(Reaction \sim Days + (1|Subject), sleepstudyNA)
## the special case of refitting with a single simulation works ...
ss0 <- refit(fm0, simulate(fm0))</pre>
## ... but if simulating multiple responses (for efficiency),
## need to use na.action=na.exclude in order to have proper length of data
fm1 <- lmer(Reaction ~ Days + (1|Subject), sleepstudyNA, na.action=na.exclude)</pre>
ss <- simulate(fm1, 5)
res2 <- refit(fm1, ss[[5]])
```

refitML

Refit a Model by Maximum Likelihood Criterion

### **Description**

Refit a (merMod) model using the maximum likelihood criterion.

# Usage

```
refitML(x, ...)
## S3 method for class 'merMod'
refitML(x, optimizer = "bobyqa", ...)
```

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### **Arguments**

X	a fitted model, usually of class "lmerMod", to be refit according to the maximum likelihood criterion.
	optional additional parameters. None are used at present.
optimizer	a string indicating the optimizer to be used.

### **Details**

This function is primarily used to get a maximum likelihood fit of a linear mixed-effects model for an anova comparison.

### Value

an object like x but fit by maximum likelihood

### See Also

refit and update.merMod for more extensive refitting.

rePos

Generator object for the rePos (random-effects positions) class

# **Description**

The generator object for the rePos class used to determine the positions and orders of random effects associated with particular random-effects terms in the model.

# Usage

```
rePos(...)
```

# **Arguments**

.. Argument list (see Note).

# Methods

```
new(mer=mer) Create a new rePos object.
```

### Note

Arguments to the new methods must be named arguments. mer, an object of class "merMod", is the only required/expected argument.

# See Also

rePos

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rePos-class

Class "rePos"

### **Description**

A reference class for determining the positions in the random-effects vector that correspond to particular random-effects terms in the model formula

### **Extends**

All reference classes extend and inherit methods from "envRefClass".

# **Examples**

```
showClass("rePos")
```

residuals.merMod

residuals of merMod objects

# **Description**

residuals of merMod objects

# Usage

```
## S3 method for class 'merMod'
residuals(object,
    type = if (isGLMM(object)) "deviance" else "response",
    scaled = FALSE, ...)

## S3 method for class 'lmResp'
residuals(object,
    type = c("working", "response", "deviance", "pearson", "partial"),
    ...)

## S3 method for class 'glmResp'
residuals(object,
    type = c("deviance", "pearson", "working", "response", "partial"),
    ...)
```

# Arguments

```
object a fitted [g]lmer (merMod) object
```

type type of residuals

scaled scale residuals by residual standard deviation (=scale parameter)?

. . . additional arguments (ignored: for method compatibility)

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### **Details**

• The default residual type varies between lmerMod and glmerMod objects: they try to mimic residuals.lm and residuals.glm respectively. In particular, the default type is "response", i.e. (observed-fitted) for lmerMod objects vs. "deviance" for glmerMod objects. type="partial" is not yet implemented for either type.

• Note that the meaning of "pearson" residuals differs between residuals.lm and residuals.lme. The former returns values scaled by the square root of user-specified weights (if any), but not by the residual standard deviation, while the latter returns values scaled by the estimated standard deviation (which will include the effects of any variance structure specified in the weights argument). To replicate lme behaviour, use type="pearson", scaled=TRUE.

sigma

Extract Residual Standard Deviation 'Sigma'

### **Description**

Extract the estimated standard deviation of the errors, the "residual standard deviation" (also misnamed the "residual standard error"), from a fitted model.

### Usage

```
## S3 method for class 'merMod'
sigma(object, ...)
```

### **Arguments**

object a fitted model.
... additional, optional arguments, passed from or to methods. (None currently in our two methods.)

### **Details**

Package **lme4** provides methods for mixed-effects models of class merMod and lists of linear models, lmList4.

#### Value

Typically a number, the estimated standard deviation of the errors ("residual standard deviation") for Gaussian models, and - less interpretably - the square root of the residual deviance per degree of freedom in more general models.

```
methods(sigma)# from R 3.3.0 on, shows methods from pkgs 'stats' *and* 'lme4'
```

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simulate.merMod

Simulate Responses From merMod Object

### **Description**

Simulate responses from a "merMod" fitted model object, i.e., from the model represented by it.

### Usage

# **Arguments**

object	(for simulate.merMod) a fitted model object or (for simulate.formula) a (one-sided) mixed model formula, as described for lmer.
nsim	positive integer scalar - the number of responses to simulate.
seed	an optional seed to be used in set.seed immediately before the simulation so as to generate a reproducible sample.
use.u	(logical) if TRUE, generate a simulation conditional on the current random-effects estimates; if FALSE generate new Normally distributed random-effects values. (Redundant with re.form, which is preferred: TRUE corresponds to re.form = NULL (condition on all random effects), while FALSE corresponds to re.form = ~0 (condition on none of the random effects).)
re.form	formula for random effects to condition on. If NULL, condition on all random effects; if NA or ~0, condition on no random effects. See Details.
ReForm, REForm,	REform
	deprecated: re.form is now the preferred argument name.
newdata	data frame for which to evaluate predictions.
newparams	new parameters to use in evaluating predictions, specified as in the start parameter for lmer or glmer – a list with components theta and beta and (for LMMs or GLMMs that estimate a scale parameter) sigma

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formula a (one-sided) mixed model formula, as described for lmer.

family a GLM family, as in glmer.

weights prior weights, as in lmer or glmer.

offset offset, as in glmer.

allow.new.levels

(logical) if FALSE (default), then any new levels (or NA values) detected in newdata will trigger an error; if TRUE, then the prediction will use the unconditional (population-level) values for data with previously unobserved levels

(or NAs).

na.action what to do with NA values in new data: see na.fail

cond.sim (experimental) simulate the conditional distribution? if FALSE, simulate only

random effects; do not simulate from the conditional distribution, rather return

the predicted group-level values

... optional additional arguments: none are used at present.

#### **Details**

ordinarily simulate is used to generate new values from an existing, fitted model (merMod object): however, if formula, newdata, and newparams are specified, simulate generates the appropriate model structure to simulate from.

• The re.form argument allows the user to specify how the random effects are incorporated in the simulation. All of the random effects terms included in re.form will be *conditioned on* that is, the conditional modes of those random effects will be included in the deterministic part of the simulation. (If new levels are used (and allow.new.levels is TRUE), the conditional modes for these levels will be set to the population mode, i.e. values of zero will be used for the random effects.) Conversely, the random effect terms that are *not* included in re.form will be *simulated from* - that is, new values will be chosen for each group based on the estimated random-effects variances.

The default behaviour (using re.form=NA) is to condition on none of the random effects, simulating new values for all of the random effects.

- For Gaussian fits, sigma specifies the residual standard deviation; for Gamma fits, it specifies the shape parameter (the rate parameter for each observation i is calculated as shape/mean(i)). For negative binomial fits, the overdispersion parameter is specified via the family, e.g. simulate(..., family=negat
- For binomial models, simulate.formula looks for the binomial size first in the weights argument (if it's supplied), second from the left-hand side of the formula (if the formula has been specified in success/failure form), and defaults to 1 if neither of those have been supplied. Simulated responses will be given as proportions, unless the supplied formula has a matrix-valued left-hand side, in which case they will be given in matrix form. If a left-hand side is given, variables in that expression must be available in newdata.
- For negative binomial models, use the negative.binomial family (from the MASS package) and specify the overdispersion parameter via the theta (sic) parameter of the family function, e.g. simulate(...,family=negative.binomial(theta=1)) to simulate from a geometric distribution (negative binomial with overdispersion parameter 1).

### See Also

bootMer for "simulestimate", i.e., where each simulation is followed by refitting the model.

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### **Examples**

```
## test whether fitted models are consistent with the
## observed number of zeros in CBPP data set:
gm1 <- glmer(cbind(incidence, size - incidence) ~ period + (1 | herd),</pre>
              data = cbpp, family = binomial)
gg <- simulate(gm1,1000)</pre>
zeros <- sapply(gg,function(x) sum(x[,"incidence"]==0))</pre>
plot(table(zeros))
abline(v=sum(cbpp$incidence==0),col=2)
## simulate from a non-fitted model; in this case we are just
## replicating the previous model, but starting from scratch
params <- list(theta=0.5,beta=c(2,-1,-2,-3))
simdat <- with(cbpp,expand.grid(herd=levels(herd),period=factor(1:4)))</pre>
simdat$size <- 15</pre>
simdat$incidence <- sample(0:1,size=nrow(simdat),replace=TRUE)</pre>
form <- formula(gm1)[-2] ## RHS of equation only</pre>
\verb|simulate| (form, newdata = \verb|simdat|, family = \verb|binomial|, \\
    newparams=params)
## simulate from negative binomial distribution instead
simulate(form, newdata=simdat, family=negative.binomial(theta=2.5),
    newparams=params)
```

sleepstudy

Reaction times in a sleep deprivation study

### **Description**

The average reaction time per day for subjects in a sleep deprivation study. On day 0 the subjects had their normal amount of sleep. Starting that night they were restricted to 3 hours of sleep per night. The observations represent the average reaction time on a series of tests given each day to each subject.

### **Format**

A data frame with 180 observations on the following 3 variables.

Reaction Average reaction time (ms)

Days Number of days of sleep deprivation

Subject Subject number on which the observation was made.

# Details

These data are from the study described in Belenky et al. (2003), for the sleep-deprived group and for the first 10 days of the study, up to the recovery period.

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### References

Gregory Belenky, Nancy J. Wesensten, David R. Thorne, Maria L. Thomas, Helen C. Sing, Daniel P. Redmond, Michael B. Russo and Thomas J. Balkin (2003) Patterns of performance degradation and restoration during sleep restriction and subsequent recovery: a sleep dose-response study. *Journal of Sleep Research* 12, 1–12.

# **Examples**

subbars

"Sub[stitute] Bars"

# **Description**

Substitute the '+' function for the 'l' function in a mixed-model formula, recursively (hence the argument name term). This provides a formula suitable for the current model.frame function.

### Usage

```
subbars(term)
```

### **Arguments**

term

a mixed-model formula

### Value

the formula with all | operators replaced by +

### See Also

```
formula, model.frame, model.matrix.

Other utilities: findbars, nobars, mkRespMod, mkReTrms, nlformula.
```

```
subbars(Reaction ~ Days + (Days|Subject)) ## => Reaction ~ Days + (Days + Subject)
```

VarCorr

troubleshooting

**Troubleshooting** 

### **Description**

This page attempts to summarize some of the common problems with fitting [gn]lmer models and how to troubleshoot them.

- failure to converge in (xxxx) evaluations The optimizer hit its maximum limit of function evaluations. To increase this, use the optControl argument of [g]lmerControl for Nelder\_Mead and bobyqa the relevant parameter is maxfun; for optim and optimx-wrapped optimizers, including nlminbwrap, it's maxit; for nloptwrap, it's maxeval.
- Model failed to converge with max|grad| ... The scaled gradient at the fitted (RE)ML estimates is worryingly large. Try
  - refitting the parameters starting at the current estimates: getting consistent results (with no warning) suggests a false positive
  - switching optimizers: getting consistent results suggests there is not really a problem; getting a similar log-likelihood with different parameter estimates suggests that the parameters are poorly determined (possibly the result of a misspecified or overfitted model)
  - compute values of the deviance in the neighbourhood of the estimated parameters to double-check that lme4 has really found a local optimum.
- Hessian is numerically singular: parameters are not uniquely determined The Hessian (inverse curvature matrix) at the maximum likelihood or REML estimates has a very large eigenvalue, indicating that (within numerical tolerances) the surface is completely flat in some direction. The model may be misspecified, or extremely badly scaled (see "Model is nearly unidentifiable").
- Model is nearly unidentifiable ... Rescale variables? The Hessian (inverse curvature matrix) at the maximum likelihood or REML estimates has a large eigenvalue, indicating that the surface is nearly flat in some direction. Consider centering and/or scaling continuous predictor variables.
- Contrasts can be applied only to factors with 2 or more levels One or more of the categorical predictors in the model has fewer than two levels. This may be due to user error when converting these predictors to factors prior to modeling, or it may result from some factor levels being eliminated due to NAs in other predictors. Double-check the number of data points in each factor level to see which one is the culprit: lapply(na.omit(df[,vars]), table) (where df is the data.frame and vars are the column names of your predictor variables).

VarCorr

Extract Variance and Correlation Components

# Description

This function calculates the estimated variances, standard deviations, and correlations between the random-effects terms in a mixed-effects model, of class merMod (linear, generalized or nonlinear). The within-group error variance and standard deviation are also calculated.

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### **Usage**

### **Arguments**

Х	for VarCorr: a fitted model object, usually an object inheriting from class merMod. For as.data.frame, a VarCorr.merMod object returned from VarCorr.
sigma	an optional numeric value used as a multiplier for the standard deviations.
digits	an optional integer value specifying the number of digits
order	arrange data frame with variances/standard deviations first and covariances/correlations last for each random effects term ("cov.last"), or in the order of the lower triangle of the variance-covariance matrix ("lower.tri")?
row.names, optional	
	Ignored: necessary for the as.data.frame method.
• • •	Ignored for the as.data.frame method; passed to other print() methods for the print() method.
comp	a character vector, specifying the components to be printed; simply passed to formatVC().
formatter	a function for formatting the numbers; simply passed to formatVC().

# Details

The print method for VarCorr.merMod objects has optional arguments digits (specify digits of precision for printing) and comp: the latter is a character vector with any combination of "Variance" and "Std.Dev.", to specify whether variances, standard deviations, or both should be printed.

### Value

An object of class VarCorr.merMod. The internal structure of the object is a list of matrices, one for each random effects grouping term. For each grouping term, the standard deviations and correlation matrices for each grouping term are stored as attributes "stddev" and "correlation", respectively, of the variance-covariance matrix, and the residual standard deviation is stored as attribute "sc" (for glmer fits, this attribute stores the scale parameter of the model).

The as.data.frame method produces a combined data frame with one row for each variance or covariance parameter (and a row for the residual error term where applicable) and the following columns:

```
grp grouping factor
```

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```
var1 first variable
var2 second variable (NA for variance parameters)
vcov variances or covariances
sdcor standard deviations or correlations
```

### Author(s)

This is modeled after VarCorr from package **nlme**, by Jose Pinheiro and Douglas Bates.

### See Also

```
1mer, nlmer
```

# **Examples**

```
data(Orthodont, package="nlme")
fm1 <- lmer(distance ~ age + (age|Subject), data = Orthodont)
(vc <- VarCorr(fm1))  ## default print method: standard dev and corr
## both variance and std.dev.
print(vc,comp=c("Variance","Std.Dev."),digits=2)
## variance only
print(vc,comp=c("Variance"))
as.data.frame(vc)
as.data.frame(vc,order="lower.tri")</pre>
```

vcconv

Convert between representations of (co-)variance structures

### **Description**

Convert between representations of (co-)variance structures (EXPERIMENTAL). See source code for details.

# Usage

```
mlist2vec(L)
vec2mlist(v, n = NULL, symm = TRUE)
vec2STlist(v, n = NULL)
sdcor2cov(m)
cov2sdcor(V)
Vv_to_Cv(v, n = NULL, s = 1)
Sv_to_Cv(v, n = NULL, s = 1)
Cv_to_Vv(v, n = NULL, s = 1)
Cv_to_Sv(v, n = NULL, s = 1)
```

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### **Arguments**

L	List of symmetric, upper-triangular, or lower-triangular square matrices.
V	Concatenated vector containing the elements of the lower-triangle (including the diagonal) of a symmetric or triangular matrix.
n	Number of rows (and columns) of the resulting matrix.
symm	Return symmetric matrix if TRUE or lower-triangular if FALSE.
m	Standard deviation-correlation matrix.
V	Covariance matrix.
s	Scale parameter.

### **Details**

- mlist2vecConvert list of matrices to concatenated vector of lower triangles with an attribute that gives the dimension of each matrix in the original list. This attribute may be used to reconstruct the matrices. Returns a concatenation of the elements in one triangle of each matrix. An attribute "clen" gives the dimension of each matrix.
- vec2mlistConvert concatenated vector to list of matrices (lower triangle or symmetric). These matrices could represent Cholesky factors, covariance matrices, or correlation matrices (with standard deviations on the diagonal).
- vec2STlistConvert concatenated vector to list of ST matrices.
- sdcor2covStandard deviation-correlation matrix to covariance matrix convert 'sdcor' format (std dev on diagonal, cor on off-diag) to and from variance-covariance matrix.
- cov2sdcorCovariance matrix to standard deviation-correlation matrix (i.e. standard deviations on the diagonal and correlations off the diagonal).
- Vv\_to\_CvVariance-covariance to relative covariance factor. Returns a vector of elements from the lower triangle of a relative covariance factor.
- Sv\_to\_CvStandard-deviation-correlation to relative covariance factor. Returns a vector of elements from the lower triangle of a relative covariance factor.
- Cv\_to\_VvRelative covariance factor to variance-covariance. From unscaled Cholesky vector to (possibly scaled) variance-covariance vector. Returns a vector of elements from the lower triangle of a variance-covariance matrix.
- Cv\_to\_SvRelative covariance factor to standard-deviation-correlation. From unscaled Chol to sd-cor vector. Returns a vector of elements from the lower triangle of a standard-deviationcorrelation matrix.

### Value

(Co-)variance structure

```
vec2mlist(1:6)
mlist2vec(vec2mlist(1:6)) # approximate inverse
```

VerbAgg

VerbAgg

Verbal Aggression item responses

### **Description**

These are the item responses to a questionaire on verbal aggression. These data are used throughout De Boeck and Wilson, *Explanatory Item Response Models* (Springer, 2004) to illustrate various forms of item response models.

### **Format**

A data frame with 7584 observations on the following 13 variables.

Anger the subject's Trait Anger score as measured on the State-Trait Anger Expression Inventory (STAXI)

Gender the subject's gender - a factor with levels M and F

item the item on the questionaire, as a factor

resp the subject's response to the item - an ordered factor with levels no < perhaps < yes

id the subject identifier, as a factor

btype behavior type - a factor with levels curse, scold and shout

situ situation type - a factor with levels other and self indicating other-to-blame and self-toblame

mode behavior mode - a factor with levels want and do

r2 dichotomous version of the response - a factor with levels N and Y

#### Source

```
http://bear.soe.berkeley.edu/EIRM/
```

### References

De Boeck and Wilson (2004), Explanatory Item Response Models, Springer.

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