

# Package ‘glmmrBase’

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**Title** Generalised Linear Mixed Models in R

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**Description** Specification, analysis, simulation, and fitting of generalised linear mixed models. Includes Markov Chain Monte Carlo Maximum likelihood and Laplace approximation model fitting for a range of models, non-linear fixed effect specifications, a wide range of flexible covariance functions that can be combined arbitrarily, robust and bias-corrected standard error estimation, power calculation, data simulation, and more. See <<https://samuel-watson.github.io/glmmr-web/>> for a detailed manual.

**License** GPL (>= 2)

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## Description

Specification, analysis, simulation, and fitting of generalised linear mixed models. Includes Markov Chain Monte Carlo Maximum likelihood and Laplace approximation model fitting for a range of models, non-linear fixed effect specifications, a wide range of flexible covariance functions that can be combined arbitrarily, robust and bias-corrected standard error estimation, power calculation, data simulation, and more. See <https://samuel-watson.github.io/glmmr-web/> for a detailed manual. `glmmrBase` provides functions for specifying, analysing, fitting, and simulating mixed models including linear, generalised linear, and models non-linear in fixed effects.

## Differences between `glmmrBase` and `lme4` and related packages.

`glmmrBase` is intended to be a broad package to support statistical work with generalised linear mixed models. While there are Laplace Approximation methods in the package, it does not intend to replace or supplant popular mixed model packages like `lme4`. Rather it provides broader functionality around simulation and analysis methods, and a range of model fitting algorithms not found in other mixed model packages. The key features are:

- Stochastic maximum likelihood methods. The most widely used methods for mixed model fitting are penalised quasi-likelihood, Laplace approximation, and Gaussian quadrature methods. These methods are widely available in other packages. We provide Markov Chain Monte Carlo (MCMC) Maximum Likelihood and Stochastic Approximation Expectation Maximisation algorithms for model fitting, with various features. These algorithms approximate the intractable GLMM likelihood using MCMC and so can provide an arbitrary level of precision. These methods may provide better maximum likelihood performance than other approximations in settings with high-dimensional or complex random effects, small sample sizes, or non-linear models.
- Flexible support for a wide range of covariance functions. The support for different covariance functions can be limited in other packages. For example, `lme4` only provides exchangeable random effects structures. We include multiple different functions that can be combined arbitrarily.
- We similarly use efficient linear algebra methods with the `Eigen` package along with `Stan` to provide MCMC sampling.
- Gaussian Process approximations. We include Hilbert Space and Nearest Neighbour Gaussian Process approximations for high dimensional random effects.
- The `Model` class includes methods for power estimation, data simulation, MCMC sampling, and calculation of a wide range of matrices and values associated with the models.
- We include natively a range of small sample corrections to information matrices, including Kenward-Roger, Box, Satterthwaite, and others, which typically require add-on packages for `lme4`.
- The package provides a flexible class system for specifying mixed models that can be incorporated into other packages and settings. The linked package `glmmrOptim` provides optimal experimental design algorithms for mixed models.

- (New in version 0.9.1) The package includes functions to replicate the functionality of **lme4**, **mcml\_lmer** and **mcml\_glmer**, which will also accept **lme4** syntax.
- (New in version 0.10.1) The package also provides mixed quantile regression models estimated using the stochastic maximum likelihood algorithms described above. These models specify an asymmetric Laplace distribution for the likelihood and integrate with the other features of the package described above.

### Package development

The package is still in development and there may still be bugs and errors. While we do not expect the general user interface to change there may be changes to the underlying library as well as new additions and functionality.

### Author(s)

Sam Watson [aut, cre]

Maintainer: Sam Watson <S.I.Watson@bham.ac.uk>

---

Beta

*Beta distribution declaration*

---

### Description

Skeleton list to declare a Beta distribution in a 'Model' object

### Usage

```
Beta(link = "logit")
```

### Arguments

`link` Name of link function. Only accepts 'logit' currently.

### Value

A list with two elements naming the family and link function

---

coef.mcml	<i>Extracts fixed effect coefficients from a mcml object</i>
-----------	--

---

**Description**

Extracts the fitted fixed effect coefficients from an 'mcml' object returned from a call of 'MCML' or 'LA' in the [Model](#) class.

**Usage**

```
## S3 method for class 'mcml'
coef(object, ...)
```

**Arguments**

object	An 'mcml' model fit.
...	Further arguments passed from other methods

**Value**

A named vector.

---

coef.Model	<i>Extracts coefficients from a Model object</i>
------------	--

---

**Description**

Extracts the coefficients from a 'Model' object.

**Usage**

```
## S3 method for class 'Model'
coef(object, ...)
```

**Arguments**

object	A 'Model' object.
...	Further arguments passed from other methods

**Value**

Fixed effect and covariance parameters extracted from the model object.

---

confint.mcml	<i>Fixed effect confidence intervals for a 'mcml' object</i>
--------------	--

---

**Description**

Returns the computed confidence intervals for a 'mcml' object.

**Usage**

```
## S3 method for class 'mcml'
confint(object, ...)
```

**Arguments**

object	A 'mcml' object.
...	Further arguments passed from other methods

**Value**

A matrix (or vector) with columns giving lower and upper confidence limits for each parameter.

---

Covariance	<i>R6 Class representing a covariance function and data</i>
------------	---

---

**Description**

R6 Class representing a covariance function and data

R6 Class representing a covariance function and data

**Details**

For the generalised linear mixed model

$$\begin{aligned}
 Y &\sim F(\mu, \sigma) \\
 \mu &= h^{-1}(X\beta + Z\gamma) \\
 \gamma &\sim MVN(0, D)
 \end{aligned}$$

where h is the link function, this class defines Z and D. The covariance is defined by a covariance function, data, and parameters. A new instance can be generated with \$new(). The class will generate the relevant matrices Z and D automatically. See [glmmrBase](#) for a detailed guide on model specification.

**\*\*Intialisation\*\*** A covariance function is specified as an additive formula made up of components with structure (1|f(j)). The left side of the vertical bar specifies the covariates in the model that have a random effects structure. The right side of the vertical bar specify the covariance function

‘f’ for that term using variable named in the data ‘j’. Covariance functions on the right side of the vertical bar are multiplied together, i.e.  $(1|f(j))*g(t)$ .

There are several common functions included for a named variable in data x. A non-exhaustive list (see `glmmrBase` for a full list): \* `gr(x)`: Indicator function (1 parameter) \* `fexp(x)`: Exponential function (2 parameters) \* `ar(x)`: AR function (2 parameters) \* `sqexp(x)`: Squared exponential (1 parameter) \* `matern(x)`: Matern function (2 parameters) \* `bessel(x)`: Modified Bessel function of the 2nd kind (1 parameter) For many 2 parameter functions, such as ‘ar’ and ‘fexp’, alternative one parameter versions are also available as ‘ar0’ and ‘fexp0’. These function omit the variance parameter and so can be used in combination with ‘gr’ functions such as ‘gr(j)\*ar0(t)’.

Parameters are provided to the covariance function as a vector. The parameters in the vector for each function should be provided in the order the covariance functions are written are written. For example, \* Formula: ‘~(1|gr(j))+(1|gr(j)\*t)’; parameters: ‘c(0.05,0.01)’ \* Formula: ‘~(1|gr(j))\*fexp0(t)’; parameters: ‘c(0.05,0.5)’

Updating of parameters is automatic if using the ‘update\_parameters()’ member function.

Using ‘update\_parameters()’ is the preferred way of updating the parameters of the mean or covariance objects as opposed to direct assignment, e.g. ‘self\$parameters <- c(...)’. The function calls check functions to automatically update linked matrices with the new parameters.

## Public fields

data Data frame with data required to build covariance

formula Covariance function formula.

parameters Model parameters specified in order of the functions in the formula.

Z Design matrix

D Covariance matrix of the random effects

## Methods

### Public methods:

- `Covariance$n()`
- `Covariance$new()`
- `Covariance$update_parameters()`
- `Covariance$print()`
- `Covariance$subset()`
- `Covariance$chol_D()`
- `Covariance$log_likelihood()`
- `Covariance$simulate_re()`
- `Covariance$sparse()`
- `Covariance$parameter_table()`
- `Covariance$nngp()`
- `Covariance$hsgp()`
- `Covariance$clone()`

**Method n():** Return the size of the design

*Usage:*

Covariance\$n()

*Returns:* Scalar

**Method** new(): Create a new Covariance object

*Usage:*

Covariance\$new(formula, data = NULL, parameters = NULL)

*Arguments:*

formula Formula describing the covariance function. See Details

data (Optional) Data frame with data required for constructing the covariance.

parameters (Optional) Vector with parameter values for the functions in the model formula.  
See Details.

*Returns:* A Covariance object

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(c1(5)*t(5)) > ind(5))
cov <- Covariance$new(formula = ~(1|gr(c1)*ar0(t)),
                      parameters = c(0.05,0.7),
                      data= df)
```

**Method** update\_parameters(): Updates the covariance parameters

*Usage:*

Covariance\$update\_parameters(parameters)

*Arguments:*

parameters A vector of parameters for the covariance function(s). See Details.

**Method** print(): Show details of Covariance object

*Usage:*

Covariance\$print()

*Arguments:*

... ignored

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(c1(5)*t(5)) > ind(5))
Covariance$new(formula = ~(1|gr(c1)*ar0(t)),
               parameters = c(0.05,0.8),
               data= df)
```

**Method** subset(): Keep specified indices and removes the rest



*Usage:*

```
Covariance$subset(index)
```

*Arguments:*

index vector of indices to keep

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(cl(10)*t(5)) > ind(10))
cov <- Covariance$new(formula = ~(1|gr(cl)*ar0(t)),
                      parameters = c(0.05,0.8),
                      data= df)

cov$subset(1:100)
```

**Method chol\_D():** Returns the Cholesky decomposition of the covariance matrix D

*Usage:*

```
Covariance$chol_D()
```

*Returns:* A matrix

**Method log\_likelihood():** The function returns the values of the multivariate Gaussian log likelihood with mean zero and covariance D for a given vector of random effect terms.

*Usage:*

```
Covariance$log_likelihood(u)
```

*Arguments:*

u Vector of random effects

*Returns:* Value of the log likelihood

**Method simulate\_re():** Simulates a set of random effects from the multivariate Gaussian distribution with mean zero and covariance D.

*Usage:*

```
Covariance$simulate_re()
```

*Returns:* A vector of random effect values

**Method sparse():** If this function is called then sparse matrix methods will be used for calculations involving D

*Usage:*

```
Covariance$sparse(sparse = TRUE, amd = TRUE)
```

*Arguments:*

sparse Logical. Whether to use sparse methods (TRUE) or not (FALSE)

amd Logical indicating whether to use and Approximate Minimum Degree algorithm to calculate an efficient permutation matrix so that the Cholesky decomposition of  $PAP^T$  is calculated rather than A.

*Returns:* None. Called for effects.

**Method** `parameter_table()`: Returns a table showing which parameters are members of which covariance function term.

*Usage:*

```
Covariance$parameter_table()
```

*Returns:* A data frame

**Method** `nngp()`: Reports or sets the parameters for the nearest neighbour Gaussian process

*Usage:*

```
Covariance$nngp(nn = NULL)
```

*Arguments:*

`nn` Integer. Number of nearest neighbours. Optional - leave as NULL to return details of the NNGP instead.

*Returns:* If 'nn' is NULL then the function will either return FALSE if not using a Nearest neighbour approximation, or TRUE and the number of nearest neighbours, otherwise it will return nothing.

**Method** `hsgp()`: Reports or sets the parameters for the Hilbert Space Gaussian process

*Usage:*

```
Covariance$hsgp(m = NULL, L = NULL)
```

*Arguments:*

`m` Integer or vector of integers. Number of basis functions per dimension. If only a single number is provided and there is more than one dimension the same number will be applied to all dimensions.

`L` Decimal. The boundary extension.

*Returns:* If 'm' and 'L' are NULL then the function will either return FALSE if not using a Hilbert space approximation, or TRUE and the number of bases functions and boundary value, otherwise it will return nothing.

**Method** `clone()`: The objects of this class are cloneable with this method.

*Usage:*

```
Covariance$clone(deep = FALSE)
```

*Arguments:*

`deep` Whether to make a deep clone.

## Examples

```
## -----
## Method `Covariance$new`
## -----

df <- nelder(~(cl(5)*t(5)) > ind(5))
cov <- Covariance$new(formula = ~(1|gr(cl)*ar0(t)),
                      parameters = c(0.05,0.7),
                      data= df)
```

```
## -----
## Method `Covariance$print`
## -----

df <- nelder(~(cl(5)*t(5)) > ind(5))
Covariance$new(formula = ~(1|gr(cl)*ar0(t)),
               parameters = c(0.05,0.8),
               data= df)

## -----
## Method `Covariance$subset`
## -----

df <- nelder(~(cl(10)*t(5)) > ind(10))
cov <- Covariance$new(formula = ~(1|gr(cl)*ar0(t)),
                     parameters = c(0.05,0.8),
                     data= df)

cov$subset(1:100)
```

---

cross\_df

*Generate crossed block structure*


---

## Description

Generate a data frame with crossed rows from two other data frames

## Usage

```
cross_df(df1, df2)
```

## Arguments

df1	data frame
df2	data frame

## Details

For two data frames 'df1' and 'df2', the function will return another data frame that crosses them, which has rows with every unique combination of the input data frames

## Value

data frame

## Examples

```
cross_df(data.frame(t=1:4), data.frame(cl=1:3))
```

`cycles`                      *Generates all the orderings of a*

---

**Description**

Given input `a`, returns a  $\text{length}(a)^2$  vector by cycling through the values of `a`

**Usage**

```
cycles(a)
```

**Arguments**

`a`                      vector

**Value**

vector

---

`family.mcml`                      *Extracts the family from a 'mcml' object.*

---

**Description**

Extracts the [family](#) from a 'mcml' object.

**Usage**

```
## S3 method for class 'mcml'  
family(object, ...)
```

**Arguments**

`object`                      A 'mcml' object.  
`...`                      Further arguments passed from other methods

**Value**

A [family](#) object.

---

family.Model	<i>Extracts the family from a 'Model' object. This information can also be accessed directly from the Model as 'Model\$family'</i>
--------------	--

---

**Description**

Extracts the [family](#) from a 'Model' object.

**Usage**

```
## S3 method for class 'Model'
family(object, ...)
```

**Arguments**

object	A 'Model' object.
...	Further arguments passed from other methods

**Value**

A [family](#) object.

---

fitted.mcml	<i>Fitted values from a 'mcml' object</i>
-------------	---

---

**Description**

Fitted values should not be generated directly from an 'mcml' object, rather fitted values should be generated using the original 'Model'. A message is printed to the user.

**Usage**

```
## S3 method for class 'mcml'
fitted(object, ...)
```

**Arguments**

object	A 'mcml' object.
...	Further arguments passed from other methods

**Value**

Nothing, called for effects, unless 'override' is TRUE, when it will return a vector of fitted values.

---

fitted.Model	<i>Extract or generate fitted values from a 'Model' object</i>
--------------	--

---

### Description

Return fitted values. Does not account for the random effects. This function is a wrapper for 'Model\$fitted()', which also provides a variety of additional options for generating fitted values from mixed models. For simulated values based on resampling random effects, see also 'Model\$sim\_data()'. To predict the values including random effects at a new location see also 'Model\$predict()'.

### Usage

```
## S3 method for class 'Model'
fitted(object, ...)
```

### Arguments

object	A 'Model' object.
...	Further arguments passed from other methods

### Value

Fitted values

---

fixed.effects	<i>Extracts the fixed effect estimates</i>
---------------	--

---

### Description

Extracts the fixed effect estimates from an mcml object returned from call of 'MCML' or 'LA' in the [Model](#) class.

### Usage

```
fixed.effects(object)
```

### Arguments

object	An 'mcml' model fit.
--------	----------------------

### Value

A named, numeric vector of fixed-effects estimates.

---

formula.mcml	<i>Extracts the formula from a 'mcml' object.</i>
--------------	---

---

**Description**

Extracts the [formula](#) from a 'mcml' object. Separate formulae are specified for the fixed and random effects in the model, either of which can be returned. The complete formula is available from the generating 'Model' object as 'Model\$formula' or 'formula(Model)'

**Usage**

```
## S3 method for class 'mcml'
formula(x, ...)
```

**Arguments**

x	A 'mcml' object.
...	Further arguments passed from other methods

**Value**

A [formula](#) object.

---

formula.Model	<i>Extracts the formula from a 'Model' object</i>
---------------	---

---

**Description**

Extracts the [formula](#) from a 'Model' object. This information can also be accessed directly from the Model as 'Model\$formula'

**Usage**

```
## S3 method for class 'Model'
formula(x, ...)
```

**Arguments**

x	A 'Model' object.
...	Further arguments passed from other methods

**Value**

A [formula](#) object.

---

hessian\_from\_formula *Automatic differentiation of formulae*

---

## Description

Exposes the automatic differentiator. Allows for calculation of Jacobian and Hessian matrices of formulae in terms of specified parameters. Formula specification is as a string. Data items are automatically multiplied by a parameter unless enclosed in parentheses.

## Usage

```
hessian_from_formula(form_, data_, colnames_, parameters_)
```

## Arguments

form_	String. Formula to differentiate specified in terms of data items and parameters. Any string not identifying a function or a data item names in 'colnames' is assumed to be a parameter.
data_	Matrix. A matrix including the data. Rows represent observations. The number of columns should match the number of items in 'colnames_'
colnames_	Vector of strings. The names of the columns of 'data_', used to match data named in the formula.
parameters_	Vector of doubles. The values of the parameters at which to calculate the derivatives. The parameters should be in the same order they appear in the formula.

## Value

A list including the jacobian and hessian matrices.

## Examples

```
# obtain the Jacobian and Hessian of the log-binomial model log-likelihood.
# The model is of data from an intervention and control group
# with n1 and n0 participants, respectively, with y1 and y0 the number of events in each group.
# The mean is exp(alpha) in the control
# group and exp(alpha + beta) in the intervention group, so that beta is the log relative risk.
hessian_from_formula(
  form_ = "(y1)*(a+b)+((n1)-(y1))*log((1-exp(a+b)))+(y0)*a+((n0)-(y0))*log((1-exp(a)))",
  data_ = matrix(c(10,100,20,100), nrow = 1),
  colnames_ = c("y1", "n1", "y0", "n0"),
  parameters_ = c(log(0.1), log(0.5)))
```



---

lme4_to_glmmr	<i>Map lme4 formula to glmmrBase formula</i>
---------------	--

---

**Description**

Returns a formula that can be used for glmmrBase Models from an lme4 input.

**Usage**

```
lme4_to_glmmr(formula, cnames)
```

**Arguments**

formula	A lme4 style formula
cnames	The column names of the data to be used. These are used to check if the specified clustering variables are in the data.

**Details**

The package lme4 uses a syntax to specify random effects as '(1|x)' where 'x' is the grouping variable. This function will modify such a formula, including those with nesting and crossing operators '/' and ':' into the glmmrBase syntax using the 'gr()' function. Not typically required by the user as it is used internally in the 'mcml\_lmer' and 'mcml\_glmer' functions.

**Value**

A formula.

**Examples**

```
df <- data.frame(c1 = 1:3, t = 4:6)
f1 <- lme4_to_glmmr(y ~ x + (1|c1/t), colnames(df))
```

---

logLik.mcml	<i>Extracts the log-likelihood from an mcml object</i>
-------------	--

---

**Description**

Extracts the final log-likelihood value from an mcml object returned from call of 'MCML' or 'LA' in the [Model](#) class. The fitting algorithm estimates the fixed effects, random effects, and covariance parameters all separately. The log-likelihood is separable in the fixed and covariance parameters, so one can return the log-likelihood for either component, or the overall log-likelihood.

**Usage**

```
## S3 method for class 'mcml'
logLik(object, fixed = TRUE, covariance = TRUE, ...)
```

**Arguments**

object	An 'mcml' model fit.
fixed	Logical whether to include the log-likelihood value from the fixed effects.
covariance	Logical whether to include the log-likelihood value from the covariance parameters.
...	Further arguments passed from other methods

**Value**

An object of class 'logLik'. If both 'fixed' and 'covariance' are FALSE then it returns NA.

---

logLik.Model	<i>Extracts the log-likelihood from an mcml object</i>
--------------	--

---

**Description**

Extracts the log-likelihood value from an 'Model' object. If no data 'y' are specified then it returns NA.

**Usage**

```
## S3 method for class 'Model'
logLik(object, ...)
```

**Arguments**

object	An 'Model' object.
...	Further arguments passed from other methods

**Value**

An object of class 'logLik'. If both 'fixed' and 'covariance' are FALSE then it returns NA.

---

match_rows	<i>Generate matrix mapping between data frames</i>
------------	--

---

### Description

For a data frames 'x' and 'target', the function will return a matrix mapping the rows of 'x' to those of 'target'.

### Usage

```
match_rows(x, target, by)
```

### Arguments

x	data.frame
target	data.frame to map to
by	vector of strings naming columns in 'x' and 'target'

### Details

'x' is a data frame with n rows and 'target' a data frame with m rows. This function will return a n times m matrix that maps the rows of 'x' to those of 'target' based on the values in the columns specified by the argument 'by'

### Value

A matrix with nrow(x) rows and nrow(target) columns

### Examples

```
df <- nelder(~(c1(10)*t(5)) > ind(10))
df_unique <- df[!duplicated(df[,c('c1', 't')]),]
match_rows(df, df_unique, c('c1', 't'))
```

---

mcmc1_glmmer	<i>lme4 style generalized linear mixed model</i>
--------------	--

---

### Description

A wrapper for Model stochastic maximum likelihood model fitting replicating lme4's syntax

**Usage**

```
mcml_glmer(
  formula,
  data,
  family,
  start = NULL,
  offset = NULL,
  verbose = 1L,
  iter.warmup = 100,
  iter.sampling = 50,
  weights = NULL,
  ...
)
```

**Arguments**

formula	A two-sided linear formula object including both the fixed and random effects specifications, see <a href="#">Details</a> .
data	A data frame containing the variables named in ‘formula’.
family	A family object expressing the distribution and link function of the model, see <a href="#">family</a> .
start	Optional. A vector of starting values for the fixed effects.
offset	Optional. A vector of offset values.
verbose	Integer, controls the level of detail printed to the console, either 0 (no output), 1 (main output), or 2 (detailed output)
iter.warmup	The number of warmup iterations for the MCMC sampling step of each iteration.
iter.sampling	The number of sampling iterations for the MCMC sampling step of each iteration.
weights	Optional. A vector of observation level weights to apply to the model fit.
...	additional arguments passed to ‘Model\$MCML()’

**Details**

This function aims to replicate the syntax of lme4’s ‘lmer’ command. The specified formula can be the standard lme4 syntax, or alternatively a glmmrBase style formula can also be used to allow for the wider range of covariance function specifications. For example both ‘y~x+(1|cl/t)’ and ‘y~x+(1|gr(cl))+(1|gr(cl)\*ar1(t))’ would be valid formulae.

**Value**

A ‘mcml’ model fit object.

**Examples**

```

#create a data frame describing a cross-sectional parallel cluster
#randomised trial
df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1
# simulate data using the Model class
df$y <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  data = df,
  family = stats::binomial()
)$sim_data()
## Not run:
fit <- mcml_glmmer(y ~ factor(t) + int - 1 + (1|cl/t), data = df, family = binomial())

## End(Not run)

```

---

mcml\_lmer

*lme4 style linear mixed model*


---

**Description**

A wrapper for Model stochastic maximum likelihood model fitting replicating lme4's syntax

**Usage**

```

mcml_lmer(
  formula,
  data,
  start = NULL,
  offset = NULL,
  verbose = 1L,
  iter.warmup = 100,
  iter.sampling = 50,
  weights = NULL,
  ...
)

```

**Arguments**

formula	A two-sided linear formula object including both the fixed and random effects specifications, see Details.
data	A data frame containing the variables named in 'formula'.
start	Optional. A vector of starting values for the fixed effects.
offset	Optional. A vector of offset values.
verbose	Integer, controls the level of detail printed to the console, either 0 (no output), 1 (main output), or 2 (detailed output)

<code>iter.warmup</code>	The number of warmup iterations for the MCMC sampling step of each iteration.
<code>iter.sampling</code>	The number of sampling iterations for the MCMC sampling step of each iteration.
<code>weights</code>	Optional. A vector of observation level weights to apply to the model fit.
<code>...</code>	additional arguments passed to <code>'Model\$MCML()'</code>

### Details

This function aims to replicate the syntax of lme4's `'lmer'` command. The specified formula can be the standard lme4 syntax, or alternatively a glmmrBase style formula can also be used to allow for the wider range of covariance function specifications. For example both `'y~x+(1|cl/t)'` and `'y~x+(1|gr(cl))+(1|gr(cl)*ar1(t))'` would be valid formulae.

### Value

A `'mcmr'` model fit object.

### Examples

```
#create a data frame describing a cross-sectional parallel cluster
#randomised trial
df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1
# simulate data using the Model class
df$y <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  data = df,
  family = stats::gaussian()
)$sim_data()
## Not run:
fit <- mcmr_lmer(y ~ factor(t) + int - 1 + (1|cl/t), data = df)

## End(Not run)
```

---

mcmr\_family

*Returns the file name and type for MCNR function*

---

### Description

Returns the file name and type for MCNR function

### Usage

```
mcmr_family(family, cmdstan)
```

**Arguments**

family	family object
cmdstan	Logical indicating whether cmdstan is being used and the function will return the filename

**Value**

list with filename and type

---

MeanFunction	<i>R6 Class representing a mean function/linear predictor</i>
--------------	---

---

**Description**

R6 Class representing a mean function/linear predictor

R6 Class representing a mean function/linear predictor

**Details**

For the generalised linear mixed model

$$Y \sim F(\mu, \sigma)$$

$$\mu = h^{-1}(X\beta + Z\gamma)$$

$$\gamma \sim MVN(0, D)$$

this class defines the fixed effects design matrix X. The mean function is defined by a model formula, data, and parameters. A new instance can be generated with `$new()`. The class will generate the relevant matrix X automatically. See [glmmrBase](#) for a detailed guide on model specification.

Specification of the mean function follows standard model formulae in R. For example for a stepped-wedge cluster trial model, a typical mean model is  $E(y_{ijt}|\delta) = \beta_0 + \tau_t + \beta_1 d_{jt} + z_{ijt}\delta$  where  $\tau_t$  are fixed effects for each time period. The formula specification for this would be `'~ factor(t) + int'` where `'int'` is the name of the variable indicating the treatment.

One can also include non-linear functions of variables in the mean function, and name the parameters. The resulting X matrix is then a matrix of first-order partial derivatives. For example, one can specify `'~ int + b_1*exp(b_2*x)'`.

Using `'update_parameters()'` is the preferred way of updating the parameters of the mean or covariance objects as opposed to direct assignment, e.g. `'self$parameters <- c(...)'`. The function calls check functions to automatically update linked matrices with the new parameters.

**Public fields**

formula model formula for the fixed effects

data Data frame with data required to build X

parameters A vector of parameter values for  $\beta$  used for simulating data and calculating covariance matrix of observations for non-linear models.

offset An optional vector specifying the offset values

X the fixed effects design matrix

**Methods****Public methods:**

- `MeanFunction$n()`
- `MeanFunction$new()`
- `MeanFunction$print()`
- `MeanFunction$update_parameters()`
- `MeanFunction$colnames()`
- `MeanFunction$subset_rows()`
- `MeanFunction$linear_predictor()`
- `MeanFunction$any_nonlinear()`
- `MeanFunction$clone()`

**Method** `n()`: Returns the number of observations

*Usage:*

```
MeanFunction$n()
```

*Arguments:*

... ignored

*Returns:* The number of observations in the model

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(c1(4)*t(5)) > ind(5))
df$int <- 0
df[df$c1 <= 2, 'int'] <- 1
mf1 <- MeanFunction$new(formula = ~ int ,
                        data=df,
                        parameters = c(-1,1)
                        )

mf1$n()
```

**Method** `new()`: Create a new MeanFunction object

*Usage:*



```
MeanFunction$new(
  formula,
  data,
  parameters = NULL,
  offset = NULL,
  verbose = FALSE
)
```

*Arguments:*

*formula* A [formula](#) object that describes the mean function, see [Details](#)

*data* (Optional) A data frame containing the covariates in the model, named in the model formula

*parameters* (Optional) A vector with the values of the parameters  $\beta$  to use in data simulation and covariance calculations. If the parameters are not specified then they are initialised to 0.

*offset* A vector of offset values (optional)

*verbose* Logical indicating whether to report detailed output

*Returns:* A MeanFunction object

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(c1(4)*t(5)) > ind(5))
df$int <- 0
df[df$c1 <= 2, 'int'] <- 1
mf1 <- MeanFunction$new(formula = ~ int ,
                        data=df,
                        parameters = c(-1,1),
                        )
```

**Method** `print()`: Prints details about the object

*Usage:*

```
MeanFunction$print()
```

*Arguments:*

... ignored

**Method** `update_parameters()`: Updates the model parameters

*Usage:*

```
MeanFunction$update_parameters(parameters)
```

*Arguments:*

*parameters* A vector of parameters for the mean function.

*verbose* Logical indicating whether to provide more detailed feedback

**Method** `colnames()`: Returns or replaces the column names of the data in the object

*Usage:*

```
MeanFunction$colnames(names = NULL)
```

*Arguments:*

names If NULL then the function prints the column names, if a vector of names, then it attempts to replace the current column names of the data

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(cl(4)*t(5)) > ind(5))
df$int <- 0
df[df$cl <= 5, 'int'] <- 1
mf1 <- MeanFunction$new(formula = ~ int ,
                        data=df,
                        parameters = c(-1,1)
                        )
mf1$colnames(c("cluster", "time", "individual", "treatment"))
mf1$colnames()
```

**Method** subset\_rows(): Keeps a subset of the data and removes the rest

All indices not in the provided vector of row numbers will be removed from both the data and fixed effects design matrix X.

*Usage:*

```
MeanFunction$subset_rows(index)
```

*Arguments:*

index Rows of the data to keep

*Returns:* NULL

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(cl(4)*t(5)) > ind(5))
df$int <- 0
df[df$cl <= 5, 'int'] <- 1
mf1 <- MeanFunction$new(formula = ~ int ,
                        data=df,
                        parameters = c(-1,1)
                        )
mf1$subset_rows(1:20)
```

**Method** linear\_predictor(): Returns the linear predictor

Returns the linear predictor,  $X * \beta$

*Usage:*

```
MeanFunction$linear_predictor()
```

*Returns:* A vector

**Method** `any_nonlinear()`: Returns a logical indicating whether the mean function contains non-linear functions of model parameters. Mainly used internally.

*Usage:*

```
MeanFunction$any_nonlinear()
```

*Returns:* None. Called for effects

**Method** `clone()`: The objects of this class are cloneable with this method.

*Usage:*

```
MeanFunction$clone(deep = FALSE)
```

*Arguments:*

`deep` Whether to make a deep clone.

## Examples

```
## -----
## Method `MeanFunction$n`
## -----

df <- nelder(~(cl(4)*t(5)) > ind(5))
df$int <- 0
df[df$cl <= 2, 'int'] <- 1
mf1 <- MeanFunction$new(formula = ~ int ,
                        data=df,
                        parameters = c(-1,1)
                        )
mf1$n()

## -----
## Method `MeanFunction$new`
## -----

df <- nelder(~(cl(4)*t(5)) > ind(5))
df$int <- 0
df[df$cl <= 2, 'int'] <- 1
mf1 <- MeanFunction$new(formula = ~ int ,
                        data=df,
                        parameters = c(-1,1),
                        )

## -----
## Method `MeanFunction$colnames`
## -----

df <- nelder(~(cl(4)*t(5)) > ind(5))
df$int <- 0
df[df$cl <= 5, 'int'] <- 1
mf1 <- MeanFunction$new(formula = ~ int ,
```

```

                                data=df,
                                parameters = c(-1,1)
                                )
mf1$colnames(c("cluster","time","individual","treatment"))
mf1$colnames()

## -----
## Method `MeanFunction$subset_rows`
## -----

df <- nelder(~(cl(4)*t(5)) > ind(5))
df$int <- 0
df[df$cl <= 5, 'int'] <- 1
mf1 <- MeanFunction$new(formula = ~ int ,
                        data=df,
                        parameters = c(-1,1)
                        )
mf1$subset_rows(1:20)

```

---

Model

*A GLMM Model*


---

### Description

A GLMM Model

A GLMM Model

### Details

A generalised linear mixed model

See [glmmrBase-package](#) for a more in-depth guide.

The generalised linear mixed model is:

$$\begin{aligned}
 Y &\sim F(\mu, \sigma) \\
 \mu &= h^{-1}(X\beta + Zu) \\
 u &\sim MVN(0, D)
 \end{aligned}$$

where  $F$  is a distribution with scale parameter

$$\sigma$$

,  $h$  is a link function,  $X$  are the fixed effects with parameters

$$\beta$$

,  $Z$  is the random effect design matrix with multivariate Gaussian distributed effects  $u$ . The class provides access to all of the elements of the model above and associated calculations and functions

including model fitting, power analysis, and various relevant matrices, including information matrices and related corrections. The object is an R6 class and so can serve as a parent class for extended functionality.

The currently support families (links) are Gaussian (identity, log), Binomial (logit, log, probit, identity), Poisson (log, identity), Gamma (logit, identity, inverse), and Beta (logit). The class also supports mixed quantile regression models, although functionality is currently experimental. Quantile models use an asymmetrical Laplace distribution for the likelihood and support all five link functions listed before.

Many calculations use the covariance matrix of the observations, such as the information matrix, which is used in power calculations and other functions. For non-Gaussian models, the class uses the first-order approximation proposed by Breslow and Clayton (1993) based on the marginal quasiliikelihood:

$$\Sigma = W^{-1} + ZDZ^T$$

where  $W$  is a diagonal matrix with the GLM iterated weights for each observation equal to, for individual  $i$   $\left(\frac{\partial h^{-1}(\eta_i)}{\partial \eta_i}\right)^2 \text{Var}(y|u)$  (see Table 2.1 in McCullagh and Nelder (1989)). The modification proposed by Zegers et al to the linear predictor to improve the accuracy of approximations based on the marginal quasiliikelihood is also available, see `use_attenuation()`.

See `glmmrBase` for a detailed guide on model specification. A detailed vignette for this package is also available online [doi:10.48550/arXiv.2303.12657](https://doi.org/10.48550/arXiv.2303.12657).

**Attenuation** For calculations such as the information matrix, the first-order approximation to the covariance matrix proposed by Breslow and Clayton (1993), described above, is used. The approximation is based on the marginal quasiliikelihood. Zegers, Liang, and Albert (1988) suggest that a better approximation to the marginal mean is achieved by "attenuating" the linear predictor. Setting `use` equal to `TRUE` uses this adjustment for calculations using the covariance matrix for non-linear models.

Calls the respective print methods of the linked covariance and mean function objects.

The matrices  $X$  and  $Z$  both have  $n$  rows, where  $n$  is the number of observations in the model/design.

Using `update_parameters()` is the preferred way of updating the parameters of the mean or covariance objects as opposed to direct assignment, e.g. `self$covariance$parameters <- c(...)`. The function calls check functions to automatically update linked matrices with the new parameters.

**Stochastic maximum likelihood** Fits generalised linear mixed models using one of several algorithms: Markov Chain Newton Raphson (MCNR), Markov Chain Expectation Maximisation (MCEM), or stochastic approximation expectation maximisation (SAEM) with or without Polyak-Ruppert averaging. MCNR and MCEM are described by McCulloch (1997) [doi:10.1080/01621459.1997.10473613](https://doi.org/10.1080/01621459.1997.10473613). For each iteration of the algorithms the unobserved random effect terms ( $\gamma$ ) are simulated using Markov Chain Monte Carlo (MCMC) methods, and then these values are conditioned on in the subsequent steps to estimate the covariance parameters and the mean function parameters ( $\beta$ ). SAEM uses a Robbins-Munroe approach to approximating the likelihood and requires fewer MCMC samples and may have lower Monte Carlo error, see Jank (2006) [doi:10.1198/106186006X157469](https://doi.org/10.1198/106186006X157469). The option `alpha` determines the rate at which successive iterations "forget" the past and must be between 0.5 and 1. Higher values will result in lower Monte Carlo error but slower convergence. The options `mcem.adapt` and `mcnr.adapt` will modify the number of MCMC samples during each step of model fitting using the suggested values in Caffo, Jank, and Jones (2006) [doi:10.1111/j.1467-9868.2005.00499.x](https://doi.org/10.1111/j.1467-9868.2005.00499.x) as the estimates converge.

The accuracy of the algorithm depends on the user specified tolerance. For higher levels of tolerance, larger numbers of MCMC samples are likely need to sufficiently reduce Monte Carlo error. However, the SAEM approach does overcome reduce the required samples, especially with R-P averaging. As such a lower number (20-50) samples per iteration is normally sufficient to get convergence.

There are several stopping rules for the algorithm. Either the algorithm will terminate when successive parameter estimates are all within a specified tolerance of each other (`conv.criterion = 1`), or when there is a high probability that the estimated log-likelihood has not been improved. This latter criterion can be applied to either the overall log-likelihood (`conv.criterion = 2`), the likelihood just for the fixed effects (`conv.criterion = 3`), or both the likelihoods for the fixed effects and covariance parameters (`conv.criterion = 4`; default).

Options for the MCMC sampler are set by changing the values in `self$mcmc_options`. The information printed to the console during model fitting can be controlled with the `self$set_trace()` function.

To provide weights for the model fitting, store them in `self$weights`. To set the number of trials for binomial models, set `self$trials`.

**Laplace approximation** Fits generalised linear mixed models using Laplace approximation to the log likelihood. For non-Gaussian models the covariance matrix is approximated using the first order approximation based on the marginal quasilielihood proposed by Breslow and Clayton (1993). The marginal mean in this approximation can be further adjusted following the proposal of Zeger et al (1988), use the member function `use_attenuated()` in this class, see [Model](#). To provide weights for the model fitting, store them in `self$weights`. To set the number of trials for binomial models, set `self$trials`. To control the information printed to the console during model fitting use the `self$set_trace()` function.

### Public fields

`covariance` A [Covariance](#) object defining the random effects covariance.

`mean` A [MeanFunction](#) object, defining the mean function for the model, including the data and covariate design matrix X.

`family` One of the family function used in R's glm functions. See [family](#) for details

`weights` A vector indicting the weights for the observations.

`trials` For binomial family models, the number of trials for each observation. The default is 1 (bernoulli).

`formula` The formula for the model. May be empty if separate formulae are specified for the mean and covariance components.

`var_par` Scale parameter required for some distributions (Gaussian, Gamma, Beta).

`mcmc_options` There are five options for MCMC sampling that are specified in this list:

- `warmup` The number of warmup iterations. Note that if using the internal HMC sampler, this only applies to the first iteration of the MCML algorithm, as the values from the previous iteration are carried over.
- `samps` The number of MCMC samples drawn in the MCML algorithms. For smaller tolerance values larger numbers of samples are required. For the internal HMC sampler, larger numbers of samples are generally required than if using Stan since the samples

generally exhibit higher autocorrelation, especially for more complex covariance structures. For SAEM a small number is recommended as all samples are stored and used from every iteration.

- `lambda` (Only relevant for the internal HMC sampler) Value of the trajectory length of the leapfrog integrator in Hamiltonian Monte Carlo (equal to number of steps times the step length). Larger values result in lower correlation in samples, but require larger numbers of steps and so is slower. Smaller numbers are likely required for non-linear GLMMs.
- `refresh` How frequently to print to console MCMC progress if displaying verbose output.
- `maxsteps` (Only relevant for the internal HMC sampler) Integer. The maximum number of steps of the leapfrog integrator

## Methods

### Public methods:

- `Model$use_attenuation()`
- `Model$fitted()`
- `Model$residuals()`
- `Model$predict()`
- `Model$new()`
- `Model$print()`
- `Model$n()`
- `Model$subset_rows()`
- `Model$sim_data()`
- `Model$update_parameters()`
- `Model$information_matrix()`
- `Model$sandwich()`
- `Model$small_sample_correction()`
- `Model$box()`
- `Model$power()`
- `Model$w_matrix()`
- `Model$dh_deta()`
- `Model$Sigma()`
- `Model$MCML()`
- `Model$LA()`
- `Model$sparse()`
- `Model$mcmc_sample()`
- `Model$gradient()`
- `Model$partial_sigma()`
- `Model$u()`
- `Model$log_likelihood()`
- `Model$calculator_instructions()`
- `Model$marginal()`
- `Model$update_y()`

- `Model$set_trace()`
- `Model$clone()`

**Method** `use_attenuation()`: Sets the model to use or not use "attenuation" when calculating the first-order approximation to the covariance matrix.

*Usage:*

```
Model$use_attenuation(use)
```

*Arguments:*

`use` Logical indicating whether to use "attenuation".

*Returns:* None. Used for effects.

**Method** `fitted()`: Return fitted values. Does not account for the random effects. For simulated values based on resampling random effects, see also `sim_data()`. To predict the values including random effects at a new location see also `predict()`.

*Usage:*

```
Model$fitted(type = "link", X, u, sample = FALSE, sample_n = 100)
```

*Arguments:*

`type` One of either "link" for values on the scale of the link function, or "response" for values on the scale of the response

`X` (Optional) Fixed effects matrix to generate fitted values

`u` (Optional) Random effects values at which to generate fitted values

`sample` Logical. If TRUE then the parameters will be re-sampled from their sampling distribution. Currently only works with existing X matrix and not user supplied matrix X and this will also ignore any provided random effects.

`sample_n` Integer. If `sample` is TRUE, then this is the number of samples.

*Returns:* Fitted values as either a vector or matrix depending on the number of samples

**Method** `residuals()`: Generates the residuals for the model

Generates one of several types of residual for the model. If `conditional = TRUE` then the residuals include the random effects, otherwise only the fixed effects are included. For `type`, there are raw, pearson, and standardized residuals. For conditional residuals a matrix is returned with each column corresponding to a sample of the random effects.

*Usage:*

```
Model$residuals(type = "standardized", conditional = TRUE)
```

*Arguments:*

`type` Either "standardized", "raw" or "pearson"

`conditional` Logical indicating whether to condition on the random effects (TRUE) or not (FALSE)

*Returns:* A matrix with either one column if conditional is false, or with number of columns corresponding to the number of MCMC samples.

**Method** `predict()`: Generate predictions at new values

Generates predicted values using a new data set to specify covariance values and values for the variables that define the covariance function. The function will return a list with the linear predictor, conditional distribution of the new random effects term conditional on the current estimates of the random effects, and some simulated values of the random effects if requested.



*Usage:*

```
Model$predict(newdata, offset = rep(0, nrow(newdata)), m = 0)
```

*Arguments:*

`newdata` A data frame specifying the new data at which to generate predictions

`offset` Optional vector of offset values for the new data

`m` Number of samples of the random effects to draw

*Returns:* A list with the linear predictor, parameters (mean and covariance matrices) for the conditional distribution of the random effects, and any random effect samples.

**Method** `new()`: Create a new Model object. Typically, a model is generated from a formula and data. However, it can also be generated from a previous model fit.

*Usage:*

```
Model$new(  
  formula,  
  covariance,  
  mean,  
  data = NULL,  
  family = NULL,  
  var_par = NULL,  
  offset = NULL,  
  weights = NULL,  
  trials = NULL,  
  model_fit = NULL  
)
```

*Arguments:*

`formula` A model formula containing fixed and random effect terms. The formula can be one way (e.g.  $\sim x + (1|gr(c1))$ ) or two-way (e.g.  $y \sim x + (1|gr(c1))$ ). One way formulae will generate a valid model enabling data simulation, matrix calculation, and power, etc. Outcome data can be passed directly to model fitting functions, or updated later using member function `update_y()`. For binomial models, either the syntax `cbind(y, n-y)` can be used for outcomes, or just `y` and the number of trials passed to the argument `trials` described below.

`covariance` (Optional) Either a [Covariance](#) object, an equivalent list of arguments that can be passed to `Covariance` to create a new object, or a vector of parameter values. At a minimum the list must specify a formula. If parameters are not included then they are initialised to 0.5.

`mean` (Optional) Either a [MeanFunction](#) object, an equivalent list of arguments that can be passed to `MeanFunction` to create a new object, or a vector of parameter values. At a minimum the list must specify a formula. If parameters are not included then they are initialised to 0.

`data` A data frame with the data required for the mean function and covariance objects. This argument can be ignored if data are provided to the covariance or mean arguments either via `Covariance` and `MeanFunction` object, or as a member of the list of arguments to both covariance and mean.

`family` A family object expressing the distribution and link function of the model, see [family](#). Currently accepts [binomial](#), [gaussian](#), [Gamma](#), [poisson](#), [Beta](#), and [Quantile](#).

`var_par` (Optional) Scale parameter required for some distributions, including Gaussian. Default is NULL.

`offset` (Optional) A vector of offset values. Optional - could be provided to the argument to mean instead.

`weights` (Optional) A vector of weights.

`trials` (Optional) For binomial family models, the number of trials for each observation. If it is not set, then it will default to 1 (a bernoulli model).

`model_fit` (optional) A mcm1 model fit resulting from a call to MCML or LA

*Returns:* A new Model class object

*Examples:*

```
\dontshow{
setParallel(FALSE)
}
#create a data frame describing a cross-sectional parallel cluster
#randomised trial
df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1
mod <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  data = df,
  family = stats::gaussian()
)

# We can also include the outcome data in the model initialisation.
# For example, simulating data and creating a new object:
df$y <- mod$sim_data()

mod <- Model$new(
  formula = y ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  data = df,
  family = stats::gaussian()
)

# Here we will specify a cohort study
df <- nelder(~ind(20) * t(6))
df$int <- 0
df[df$t > 3, 'int'] <- 1

des <- Model$new(
  formula = ~ int + (1|gr(ind)),
  data = df,
  family = stats::poisson()
)

# or with parameter values specified
```

```

des <- Model$new(
  formula = ~ int + (1|gr(ind)),
  covariance = c(0.05),
  mean = c(1,0.5),
  data = df,
  family = stats::poisson()
)

#an example of a spatial grid with two time points

df <- nelder(~ (x(10)*y(10))*t(2))
spt_design <- Model$new(formula = ~ 1 + (1|ar0(t))*fexp(x,y)),
                    data = df,
                    family = stats::gaussian())

# A quantile regression model for the 25th percentile (experimental)
df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1

qmod <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  data = df,
  family = Quantile(link = "identity", scaled = TRUE, q = 0.25)
)

```

**Method** `print()`: Print method for Model class

*Usage:*

```
Model$print()
```

*Arguments:*

... ignored

**Method** `n()`: Returns the number of observations in the model

*Usage:*

```
Model$n(...)
```

*Arguments:*

... ignored

**Method** `subset_rows()`: Subsets the design keeping specified observations only

Given a vector of row indices, the corresponding rows will be kept and the other rows will be removed from the mean function and covariance

*Usage:*

```
Model$subset_rows(index)
```

*Arguments:*

`index` Integer or vector integers listing the rows to keep

*Returns:* The function updates the object and nothing is returned.

**Method** `sim_data()`: Generates a realisation of the design

Generates a single vector of outcome data based upon the specified GLMM design.

*Usage:*

```
Model$sim_data(type = "y")
```

*Arguments:*

`type` Either 'y' to return just the outcome data, 'data' to return a data frame with the simulated outcome data alongside the model data, or 'all', which will return a list with simulated outcomes `y`, matrices `X` and `Z`, parameters `beta`, and the values of the simulated random effects.

*Returns:* Either a vector, a data frame, or a list

*Examples:*

```
df <- nelder(~(c1(10)*t(5)) > ind(10))
df$int <- 0
df[df$c1 > 5, 'int'] <- 1
\dontshow{
setParallel(FALSE) # for the CRAN check
}
des <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(c1)*ar0(t)),
  covariance = c(0.05,0.8),
  mean = c(rep(0,5),0.6),
  data = df,
  family = stats::binomial()
)
ysim <- des$sim_data()
```

**Method** `update_parameters()`: Updates the parameters of the mean function and/or the covariance function

*Usage:*

```
Model$update_parameters(mean.pars = NULL, cov.pars = NULL, var.par = NULL)
```

*Arguments:*

`mean.pars` (Optional) Vector of new mean function parameters

`cov.pars` (Optional) Vector of new covariance function(s) parameters

`var.par` (Optional) A scalar value for `var_par`

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(c1(10)*t(5)) > ind(10))
df$int <- 0
df[df$c1 > 5, 'int'] <- 1
des <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(c1)*ar0(t)),
  data = df,
  family = stats::binomial()
```

```
)
des$update_parameters(cov.pars = c(0.1,0.9))
```

**Method** `information_matrix()`: Generates the information matrix of the mixed model GLS estimator ( $X'S^{-1}X$ ). The inverse of this matrix is an estimator for the variance-covariance matrix of the fixed effect parameters. For various small sample corrections see `small_sample_correction()` and `box()`. For models with non-linear functions of fixed effect parameters, a correction to the Hessian matrix is required, which is automatically calculated or optionally returned or disabled.

*Usage:*

```
Model$information_matrix(
  include.re = FALSE,
  theta = FALSE,
  hessian.corr = "add",
  adj.nonspd = TRUE
)
```

*Arguments:*

`include.re` logical indicating whether to return the information matrix including the random effects components (TRUE), or the mixed model information matrix for beta only (FALSE).

`theta` Logical. If TRUE the function will return the variance-covariance matrix for the covariance parameters and ignore the first argument. Otherwise, the fixed effect parameter information matrix is returned.

`hessian.corr` String. If there are non-linear functions of fixed effect parameters then a correction to the Hessian can be applied ("add"), returned on its own ("return"), or ignored ("none")

`adj.nonspd` Logical. For models nonlinear in fixed effect parameters, the Hessian of the linear predictor with respect to the model parameters is often not positive semi-definite, which can cause a singular matrix and failure to calculate valid standard errors. The adjustment matrix will be corrected if it is not positive semi-definite and this option is TRUE.

*Returns:* A matrix

**Method** `sandwich()`: Returns the robust sandwich variance-covariance matrix for the fixed effect parameters

*Usage:*

```
Model$sandwich()
```

*Returns:* A PxP matrix

**Method** `small_sample_correction()`: Returns a small sample correction. The option "KR" returns the Kenward-Roger bias-corrected variance-covariance matrix for the fixed effect parameters and degrees of freedom. Option "KR2" returns an improved correction given in Kenward & Roger (2009) [doi:j.csda.2008.12.013](https://doi.org/10.1080/01621459.2008.12.013). Note, that the corrected/improved version is invariant under reparameterisation of the covariance, and it will also make no difference if the covariance is linear in parameters. Exchangeable covariance structures in this package (i.e. `gr()`) are parameterised in terms of the variance rather than standard deviation, so the results will be unaffected. Option "sat" returns the "Satterthwaite" correction, which only includes corrected degrees of freedom, along with the GLS standard errors.

*Usage:*

```
Model$small_sample_correction(type)
```

*Arguments:*

type Either "KR", "KR2", or "sat", see description.

*Returns:* A PxP matrix

**Method** `box()`: Returns the inferential statistics (F-stat, p-value) for a modified Box correction [doi:10.1002/sim.4072](https://doi.org/10.1002/sim.4072) for Gaussian-identity models.

*Usage:*

```
Model$box(y)
```

*Arguments:*

y Optional. If provided, will update the vector of outcome data. Otherwise it will use the data from the previous model fit.

*Returns:* A data frame.

**Method** `power()`: Estimates the power of the design described by the model using the square root of the relevant element of the GLS variance matrix:

$$(X^T \Sigma^{-1} X)^{-1}$$

Note that this is equivalent to using the "design effect" for many models.

*Usage:*

```
Model$power(alpha = 0.05, two.sided = TRUE, alternative = "pos")
```

*Arguments:*

alpha Numeric between zero and one indicating the type I error rate. Default of 0.05.

two.sided Logical indicating whether to use a two sided test

alternative For a one-sided test whether the alternative hypothesis is that the parameter is positive "pos" or negative "neg"

*Returns:* A data frame describing the parameters, their values, expected standard errors and estimated power.

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
df <- nelder(~(c1(10)*t(5)) > ind(10))
df$int <- 0
df[df$c1 > 5, 'int'] <- 1
des <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(c1)) + (1|gr(c1,t)),
  covariance = c(0.05,0.1),
  mean = c(rep(0,5),0.6),
  data = df,
  family = stats::gaussian(),
  var_par = 1
)
des$power() #power of 0.90 for the int parameter
```

**Method** `w_matrix()`: Returns the diagonal of the matrix  $W$  used to calculate the covariance matrix approximation

*Usage:*

```
Model$w_matrix()
```

*Returns:* A vector with values of the glm iterated weights

**Method** `dh_deta()`: Returns the derivative of the link function with respect to the linear predictor

*Usage:*

```
Model$dh_deta()
```

*Returns:* A vector

**Method** `Sigma()`: Returns the (approximate) covariance matrix of  $y$   
Returns the covariance matrix  $\Sigma$ . For non-linear models this is an approximation. See Details.

*Usage:*

```
Model$Sigma(inverse = FALSE)
```

*Arguments:*

`inverse` Logical indicating whether to provide the covariance matrix or its inverse

*Returns:* A matrix.

**Method** `MCML()`: Stochastic Maximum Likelihood model fitting

*Usage:*

```
Model$MCML(  
  y = NULL,  
  method = "saem",  
  tol = 0.01,  
  max.iter = 50,  
  se = "gls",  
  mcmc.pkg = "rstan",  
  se.theta = TRUE,  
  algo = ifelse(self$mean$any_nonlinear(), 2, 3),  
  lower.bound = NULL,  
  upper.bound = NULL,  
  lower.bound.theta = NULL,  
  upper.bound.theta = NULL,  
  alpha = 0.8,  
  convergence.prob = 0.95,  
  pr.average = FALSE,  
  conv.criterion = 2  
)
```

*Arguments:*

`y` Optional. A numeric vector of outcome data. If this is not provided then either the outcome must have been specified when initialising the Model object, or the outcome data has been updated using member function `update_y()`

- method The MCML algorithm to use, either `mcm` or `mcnr`, or `saem` see Details. Default is `saem`. `mcm.adapt` and `mcnr.adapt` will use adaptive MCMC sample sizes starting small and increasing to the the maximum value specified in `mcmc_options$sampling`, which results in faster convergence. `saem` uses a stochastic approximation expectation maximisation algorithm. MCMC samples are kept from all iterations and so a smaller number of samples are needed per iteration.
- `tol` Numeric value, tolerance of the MCML algorithm, the maximum difference in parameter estimates between iterations at which to stop the algorithm. If two values are provided then different tolerances will be applied to the fixed effect and covariance parameters.
- `max.iter` Integer. The maximum number of iterations of the MCML algorithm.
- `se` String. Type of standard error and/or inferential statistics to return. Options are "gls" for GLS standard errors (the default), "robust" for robust standard errors, "kr" for original Kenward-Roger bias corrected standard errors, "kr2" for the improved Kenward-Roger correction, "sat" for Satterthwaite degrees of freedom correction (this is the same degrees of freedom correction as Kenward-Roger, but with GLS standard errors), "box" to use a modified Box correction (does not return confidence intervals), "bw" to use GLS standard errors with a between-within correction to the degrees of freedom, "bwrobust" to use robust standard errors with between-within correction to the degrees of freedom.
- `mcmc.pkg` String. Either `cmdstan` for `cmdstan` (requires the package `cmdstanr`), `rstan` to use `rstan` sampler, or `hmc` to use a cruder Hamiltonian Monte Carlo sampler. `cmdstan` is recommended as it has by far the best number of effective samples per unit time. `cmdstanr` will compile the MCMC programs to the library folder the first time they are run, so may not currently be an option for some users.
- `se.theta` Logical. Whether to calculate the standard errors for the covariance parameters. This step is a slow part of the calculation, so can be disabled if required in larger models. Has no effect for Kenward-Roger standard errors.
- `algo` Integer. 1 = L-BFGS for beta and BOBYQA for theta, 2 = BOBYQA for both, 3 = L-BFGS for both (default). The L-BFGS algorithm may perform poorly with some covariance structures, in this case select 1 or 2, or apply an upper bound.
- `lower.bound` Optional. Vector of lower bounds for the fixed effect parameters. To apply bounds use MCEM.
- `upper.bound` Optional. Vector of upper bounds for the fixed effect parameters. To apply bounds use MCEM.
- `lower.bound.theta` Optional. Vector of lower bounds for the covariance parameters (default is 0; negative values will cause an error)
- `upper.bound.theta` Optional. Vector of upper bounds for the covariance parameters.
- `alpha` If using SAEM then this parameter controls the step size. On each iteration  $i$  the step size is  $(1/\alpha)^i$ , default is 0.8. Values around 0.5 will result in lower bias but slower convergence, values closer to 1 will result in higher convergence but potentially higher error.
- `convergence.prob` Numeric value in (0,1) indicating the probability of convergence if using convergence criteria 2, 3, or 4.
- `pr.average` Logical indicating whether to use Polyak-Ruppert averaging if using the SAEM algorithm (default is TRUE)
- `conv.criterion` Integer. The convergence criterion for the algorithm. 1 = the maximum difference between parameter estimates between iterations as defined by `tol`, 2 = The probability of improvement in the overall log-likelihood is less than  $1 - \text{convergence.prob}$  3



= The probability of improvement in the log-likelihood for the fixed effects is less than 1 - convergence.prob  
 4 = The probabilities of improvement in the log-likelihood the fixed effects and covariance parameters are both less than 1 - convergence.prob

*Returns:* A mcml object

*Examples:*

```
\dontrun{
#create example data with six clusters, five time periods, and five people per cluster-period
df <- nelder(~(cl(6)*t(5)) > ind(5))
# parallel trial design intervention indicator
df$int <- 0
df[df$cl > 3, 'int'] <- 1
# specify parameter values in the call for the data simulation below
des <- Model$new(
  formula= ~ factor(t) + int - 1 +(1|gr(cl))*ar0(t)),
  covariance = c(0.05,0.7),
  mean = c(rep(0,5),0.2),
  data = df,
  family = gaussian()
)
ysim <- des$sim_data() # simulate some data from the model
fit1 <- des$MCML(y = ysim) # Default model fitting with SAEM-PR
# use MCEM instead and stop when parameter values are within 1e-2 on successive iterations
fit2 <- des$MCML(y = ysim, method="mcem",tol=1e-2,conv.criterion = 1)
}
```

**Method LA():** Maximum Likelihood model fitting with Laplace Approximation

*Usage:*

```
Model$LA(
  y = NULL,
  start,
  method = "nr",
  se = "gls",
  max.iter = 40,
  tol = 1e-04,
  se.theta = TRUE,
  algo = 2,
  lower.bound = NULL,
  upper.bound = NULL,
  lower.bound.theta = NULL,
  upper.bound.theta = NULL
)
```

*Arguments:*

*y* Optional. A numeric vector of outcome data. If this is not provided then either the outcome must have been specified when initialising the Model object, or the outcome data has been updated using member function `update_y()`

*start* Optional. A numeric vector indicating starting values for the model parameters.

method String. Either "nloptim" for non-linear optimisation, or "nr" for Newton-Raphson (default) algorithm

se String. Type of standard error and/or inferential statistics to return. Options are "gls" for GLS standard errors (the default), "robust" for robust standard errors, "kr" for original Kenward-Roger bias corrected standard errors, "kr2" for the improved Kenward-Roger correction, "sat" for Satterthwaite degrees of freedom correction (this is the same degrees of freedom correction as Kenward-Roger, but with GLS standard errors) "box" to use a modified Box correction (does not return confidence intervals), "bw" to use GLS standard errors with a between-within correction to the degrees of freedom, "bwrobust" to use robust standard errors with between-within correction to the degrees of freedom. Note that Kenward-Roger assumes REML estimates, which are not currently provided by this function.

max.iter Maximum number of algorithm iterations, default 20.

tol Maximum difference between successive iterations at which to terminate the algorithm

se.theta Logical. Whether to calculate the standard errors for the covariance parameters. This step is a slow part of the calculation, so can be disabled if required in larger models. Has no effect for Kenward-Roger standard errors.

algo Integer. 1 = L-BFGS for beta-u and BOBYQA for theta (default), 2 = BOBYQA for both.

lower.bound Optional. Vector of lower bounds for the fixed effect parameters. To apply bounds use nloptim.

upper.bound Optional. Vector of upper bounds for the fixed effect parameters. To apply bounds use nloptim.

lower.bound.theta Optional. Vector of lower bounds for the covariance parameters.

upper.bound.theta Optional. Vector of upper bounds for the covariance parameters.

*Returns:* A mcml object

*Examples:*

```
\dontshow{
setParallel(FALSE) # for the CRAN check
}
#create example data with six clusters, five time periods, and five people per cluster-period
df <- nelder(~(cl(6)*t(5)) > ind(5))
# parallel trial design intervention indicator
df$int <- 0
df[df$cl > 3, 'int'] <- 1
# specify parameter values in the call for the data simulation below
des <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl))*ar0(t),
  covariance = c(0.05,0.7),
  mean = c(rep(0,5),-0.2),
  data = df,
  family = stats::binomial()
)
ysim <- des$sim_data() # simulate some data from the model
fit1 <- des$LA(y = ysim)
```

**Method** sparse(): Set whether to use sparse matrix methods for model calculations and fitting. By default the model does not use sparse matrix methods.

*Usage:*

```
Model$sparse(sparse = TRUE, amd = TRUE)
```

*Arguments:*

`sparse` Logical indicating whether to use sparse matrix methods

`amd` Logical indicating whether to use and Approximate Minimum Degree algorithm to calculate an efficient permutation matrix so that the Cholesky decomposition of  $PAP^T$  is calculated rather than  $A$ .

*Returns:* None, called for effects

**Method** `mcmc_sample()`: Generate an MCMC sample of the random effects

*Usage:*

```
Model$mcmc_sample(mcmc.pkg = "rstan")
```

*Arguments:*

`mcmc.pkg` String. Either `cmdstan` for `cmdstan` (requires the package `cmdstanr`), `rstan` to use `rstan` sampler, or `hmc` to use a cruder Hamiltonian Monte Carlo sampler. `cmdstan` is recommended as it has by far the best number of effective samples per unit time. `cmdstanr` will compile the MCMC programs to the library folder the first time they are run, so may not currently be an option for some users.

*Returns:* A matrix of samples of the random effects

**Method** `gradient()`: The gradient of the log-likelihood with respect to either the random effects or the model parameters. The random effects are on the  $N(0,I)$  scale, i.e. scaled by the Cholesky decomposition of the matrix  $D$ . To obtain the random effects from the last model fit, see member function `$u`

*Usage:*

```
Model$gradient(y, u, beta = FALSE)
```

*Arguments:*

`y` (optional) Vector of outcome data, if not specified then data must have been set in another function.

`u` (optional) Vector of random effects scaled by the Cholesky decomposition of  $D$

`beta` Logical. Whether the log gradient for the random effects (`FALSE`) or for the linear predictor parameters (`TRUE`)

*Returns:* A vector of the gradient

**Method** `partial_sigma()`: The partial derivatives of the covariance matrix  $\Sigma$  with respect to the covariance parameters. The function returns a list in order:  $\Sigma$ , first order derivatives, second order derivatives. The second order derivatives are ordered as the lower-triangular matrix in column major order. Letting `'d(i)'` mean the first-order partial derivative with respect to parameter  $i$ , and `d2(i,j)` mean the second order derivative with respect to parameters  $i$  and  $j$ , then if there were three covariance parameters the order of the output would be: (`sigma`, `d(1)`, `d(2)`, `d(3)`, `d2(1,1)`, `d2(1,2)`, `d2(1,3)`, `d2(2,2)`, `d2(2,3)`, `d2(3,3)`).

*Usage:*

```
Model$partial_sigma()
```

*Returns:* A list of matrices, see description for contents of the list.

**Method** `u()`: Returns the sample of random effects from the last model fit, or updates the samples for the model.

*Usage:*

```
Model$u(scaled = TRUE, u)
```

*Arguments:*

`scaled` Logical indicating whether the samples are on the  $N(0,I)$  scale (`scaled=FALSE`) or  $N(0,D)$  scale (`scaled=TRUE`)

`u` (optional) Matrix of random effect samples. If provided then the internal samples are replaced with these values. These samples should be  $N(0,I)$ .

*Returns:* A matrix of random effect samples

**Method** `log_likelihood()`: The log likelihood for the GLMM. The random effects can be left unspecified. If no random effects are provided, and there was a previous model fit with the same data `y` then the random effects will be taken from that model. If there was no previous model fit then the random effects are assumed to be all zero.

*Usage:*

```
Model$log_likelihood(y, u)
```

*Arguments:*

`y` A vector of outcome data

`u` An optional matrix of random effect samples. This can be a single column.

*Returns:* The log-likelihood of the model parameters

**Method** `calculator_instructions()`: Prints the internal instructions and data used to calculate the linear predictor. Internally the class uses a reverse polish notation to store and calculate different functions, including user-specified non-linear mean functions. This function will print all the steps. Mainly used for debugging and determining how the class has interpreted non-linear model specifications.

*Usage:*

```
Model$calculator_instructions()
```

*Returns:* None. Called for effects.

**Method** `marginal()`: Calculates the marginal effect of variable `x`. There are several options for marginal effect and several types of conditioning or averaging. The type of marginal effect can be the derivative of the mean with respect to `x` (`dydx`), the expected difference  $E(y|x=a) - E(y|x=b)$  (`diff`), or the expected log ratio  $\log(E(y|x=a)/E(y|x=b))$  (`ratio`). Other fixed effect variables can be set at specific values (`at`), set at their mean values (`atmeans`), or averaged over (`average`). Averaging over a fixed effects variable here means using all observed values of the variable in the relevant calculation. The random effects can similarly be set at their estimated value (`re="estimated"`), set to zero (`re="zero"`), set to a specific value (`re="at"`), or averaged over (`re="average"`). Estimates of the expected values over the random effects are generated using MCMC samples. MCMC samples are generated either through MCML model fitting or using `mcmc_sample`. In the absence of samples `average` and `estimated` will produce the same result. The standard errors are calculated using the delta method with one of several options for the variance matrix of the fixed effect parameters. Several of the arguments require the names of the variables as given to the model object. Most variables are as specified in the formula, factor variables are specified as the name of the `variable_value`, e.g. `t_1`. To see the names of the stored parameters and data variables see the member function `names()`.

*Usage:*

```
Model$Marginal(
  x,
  type,
  re,
  se,
  at = c(),
  atmeans = c(),
  average = c(),
  xvals = c(1, 0),
  atvals = c(),
  revals = c()
)
```

*Arguments:*

- x String. Name of the variable to calculate the marginal effect for.
- type String. Either dydx for derivative, diff for difference, or ratio for log ratio. See description.
- re String. Either estimated to condition on estimated values, zero to set to zero, at to provide specific values, or average to average over the random effects.
- se String. Type of standard error to use, either GLS for the GLS standard errors, KR for Kenward-Roger estimated standard errors, KR2 for the improved Kenward-Roger correction (see `small_sample_correction()`), or robust to use a robust sandwich estimator.
- at Optional. A vector of strings naming the fixed effects for which a specified value is given.
- atmeans Optional. A vector of strings naming the fixed effects that will be set at their mean value.
- average Optional. A vector of strings naming the fixed effects which will be averaged over.
- xvals Optional. A vector specifying the values of a and b for diff and ratio. The default is (1,0).
- atvals Optional. A vector specifying the values of fixed effects specified in at (in the same order).
- revals Optional. If re="at" then this argument provides a vector of values for the random effects.

*Returns:* A named vector with elements margin specifying the point estimate and se giving the standard error.

**Method** `update_y()`: Updates the outcome data y

Some functions require outcome data, which is by default set to all zero if no model fitting function has been run. This function can update the interval y data.

*Usage:*

```
Model$update_y(y)
```

*Arguments:*

- y Vector of outcome data

*Returns:* None. Called for effects

**Method** `set_trace()`: Controls the information printed to the console for other functions.

*Usage:*

```
Model$set_trace(trace)
```

*Arguments:*

trace Integer, either 0 = no information, 1 = some information, 2 = all information

*Returns:* None. Called for effects.

**Method** clone(): The objects of this class are cloneable with this method.

*Usage:*

```
Model$clone(deep = FALSE)
```

*Arguments:*

deep Whether to make a deep clone.

**References**

Breslow, N. E., Clayton, D. G. (1993). Approximate Inference in Generalized Linear Mixed Models. *Journal of the American Statistical Association*, 88(421), 9–25. doi:10.1080/01621459.1993.10594284

McCullagh P, Nelder JA (1989). *Generalized linear models*, 2nd Edition. Routledge.

McCulloch CE (1997). “Maximum Likelihood Algorithms for Generalized Linear Mixed Models.” *Journal of the American statistical Association*, 92(437), 162–170. doi:10.2307/2291460

Zeger, S. L., Liang, K.-Y., Albert, P. S. (1988). Models for Longitudinal Data: A Generalized Estimating Equation Approach. *Biometrics*, 44(4), 1049. doi:10.2307/2531734

**See Also**

[nelder](#), [MeanFunction](#), [Covariance](#)

[Model](#), [Covariance](#), [MeanFunction](#)

[Model](#), [Covariance](#), [MeanFunction](#)

**Examples**

```
## -----
## Method `Model$new`
## -----

#create a data frame describing a cross-sectional parallel cluster
#randomised trial
df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1
mod <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  data = df,
  family = stats::gaussian()
)
```

```

# We can also include the outcome data in the model initialisation.
# For example, simulating data and creating a new object:
df$y <- mod$sim_data()

mod <- Model$new(
  formula = y ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  data = df,
  family = stats::gaussian()
)

# Here we will specify a cohort study
df <- nelder(~ind(20) * t(6))
df$int <- 0
df[df$t > 3, 'int'] <- 1

des <- Model$new(
  formula = ~ int + (1|gr(ind)),
  data = df,
  family = stats::poisson()
)

# or with parameter values specified

des <- Model$new(
  formula = ~ int + (1|gr(ind)),
  covariance = c(0.05),
  mean = c(1,0.5),
  data = df,
  family = stats::poisson()
)

#an example of a spatial grid with two time points

df <- nelder(~ (x(10)*y(10))*t(2))
spt_design <- Model$new(formula = ~ 1 + (1|ar0(t))*fexp(x,y),
  data = df,
  family = stats::gaussian())

# A quantile regression model for the 25th percentile (experimental)
df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1

qmod <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  data = df,
  family = Quantile(link = "identity", scaled = TRUE, q = 0.25)
)

## -----
## Method `Model$sim_data`
## -----

```

```

df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1

des <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl))*ar0(t),
  covariance = c(0.05,0.8),
  mean = c(rep(0,5),0.6),
  data = df,
  family = stats::binomial()
)
ysim <- des$sim_data()

## -----
## Method `Model$update_parameters`
## -----

df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1
des <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl))*ar0(t),
  data = df,
  family = stats::binomial()
)
des$update_parameters(cov.pars = c(0.1,0.9))

## -----
## Method `Model$power`
## -----

df <- nelder(~(cl(10)*t(5)) > ind(10))
df$int <- 0
df[df$cl > 5, 'int'] <- 1
des <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(cl)) + (1|gr(cl,t)),
  covariance = c(0.05,0.1),
  mean = c(rep(0,5),0.6),
  data = df,
  family = stats::gaussian(),
  var_par = 1
)
des$power() #power of 0.90 for the int parameter

## -----
## Method `Model$MCMC`
## -----

## Not run:
#create example data with six clusters, five time periods, and five people per cluster-period
df <- nelder(~(cl(6)*t(5)) > ind(5))

```



```

# parallel trial design intervention indicator
df$int <- 0
df[df$c1 > 3, 'int'] <- 1
# specify parameter values in the call for the data simulation below
des <- Model$new(
  formula= ~ factor(t) + int - 1 +(1|gr(c1)*ar0(t)),
  covariance = c(0.05,0.7),
  mean = c(rep(0,5),0.2),
  data = df,
  family = gaussian()
)
ysim <- des$sim_data() # simulate some data from the model
fit1 <- des$MCMC(y = ysim) # Default model fitting with SAEM-PR
# use MCEM instead and stop when parameter values are within 1e-2 on successive iterations
fit2 <- des$MCMC(y = ysim, method="mcem",tol=1e-2,conv.criterion = 1)

## End(Not run)

## -----
## Method `Model$LA`
## -----

#create example data with six clusters, five time periods, and five people per cluster-period
df <- nelder(~(c1(6)*t(5)) > ind(5))
# parallel trial design intervention indicator
df$int <- 0
df[df$c1 > 3, 'int'] <- 1
# specify parameter values in the call for the data simulation below
des <- Model$new(
  formula = ~ factor(t) + int - 1 + (1|gr(c1)*ar0(t)),
  covariance = c(0.05,0.7),
  mean = c(rep(0,5),-0.2),
  data = df,
  family = stats::binomial()
)
ysim <- des$sim_data() # simulate some data from the model
fit1 <- des$LA(y = ysim)

```

---

nelder

*Generates a block experimental structure using Nelder's formula*


---

### Description

Generates a data frame expressing a block experimental structure using Nelder's formula

### Usage

```
nelder(formula)
```

**Arguments**

formula            A model formula. See details

**Details**

Nelder (1965) suggested a simple notation that could express a large variety of different blocked designs. The function `nelder()` that generates a data frame of a design using the notation. There are two operations:

`'>'` (or  $\rightarrow$  in Nelder's notation) indicates "clustered in".

`'**'` (or  $\times$  in Nelder's notation) indicates a crossing that generates all combinations of two factors.

The implementation of this notation includes a string indicating the name of the variable and a number for the number of levels, such as `'abc(12)'`. So for example `'~cl(4) > ind(5)'` means in each of five levels of `'cl'` there are five levels of `'ind'`, and the individuals are different between clusters. The formula `'~cl(4) * t(3)'` indicates that each of the four levels of `'cl'` are observed for each of the three levels of `'t'`. Brackets are used to indicate the order of evaluation. Some specific examples:

`'~person(5) * time(10)'`: A cohort study with five people, all observed in each of ten periods `'time'`

`'~(cl(4) * t(3)) > ind(5)'`: A repeated-measures cluster study with four clusters (labelled `'cl'`), each observed in each time period `'t'` with cross-sectional sampling and five individuals (labelled `'ind'`) in each cluster-period.

`'~(cl(4) > ind(5)) * t(3)'`: A repeated-measures cluster cohort study with four clusters (labelled `'cl'`) with five individuals per cluster, and each cluster-individual combination is observed in each time period `'t'`.

`'~((x(100) * y(100)) > hh(4)) * t(2)'`: A spatio-temporal grid of 100x100 and two time points, with 4 households per spatial grid cell.

**Value**

A list with the first member being the data frame

**Examples**

```
nelder(~(j(4) * t(5)) > i(5))
nelder(~person(5) * time(10))
```

---

```
nest_df
```

```
Generate nested block structure
```

---

**Description**

Generate a data frame that nests one data frame in another

**Usage**

```
nest_df(df1, df2)
```

**Arguments**

df1	data frame
df2	data frame

**Details**

For two data frames 'df1' and 'df2', the function will return another data frame that nests 'df2' in 'df1'. So each row of 'df1' will be duplicated 'nrow(df2)' times and matched with 'df2'. The values of each 'df2' will be unique for each row of 'df1'

**Value**

data frame

**Examples**

```
nest_df(data.frame(t=1:4),data.frame(c1=1:3))
```

---

predict.mcml

*Predict from a 'mcml' object*

---

**Description**

Predictions cannot be generated directly from an 'mcml' object, rather new predictions should be generated using the original 'Model'. A message is printed to the user.

**Usage**

```
## S3 method for class 'mcml'  
predict(object, ...)
```

**Arguments**

object	A 'mcml' object.
...	Further arguments passed from other methods

**Value**

Nothing. Called for effects.

---

predict.Model                      *Generate predictions at new values from a 'Model' object*

---

### Description

Generates predicted values from a 'Model' object using a new data set to specify covariance values and values for the variables that define the covariance function. The function will return a list with the linear predictor, conditional distribution of the new random effects term conditional on the current estimates of the random effects, and some simulated values of the random effects if requested. Typically this functionality is accessed using 'Model\$predict()', which this function provides a wrapper for.

### Usage

```
## S3 method for class 'Model'
predict(object, newdata, offset = rep(0, nrow(newdata)), m = 0, ...)
```

### Arguments

object	A 'Model' object.
newdata	A data frame specifying the new data at which to generate predictions
offset	Optional vector of offset values for the new data
m	Number of samples of the random effects to draw
...	Further arguments passed from other methods

### Value

A list with the linear predictor, parameters (mean and covariance matrices) for the conditional distribution of the random effects, and any random effect samples.

---

print.mcml                      *Prints an mcml fit output*

---

### Description

Print method for class "'mcml'"

### Usage

```
## S3 method for class 'mcml'
print(x, ...)
```

**Arguments**

x                    an object of class "'mcml'" as a result of a call to MCML, see [Model](#)  
 ...                    Further arguments passed from other methods

**Details**

'print.mcml' tries to replicate the output of other regression functions, such as 'lm' and 'lmer' reporting parameters, standard errors, and z- and p- statistics. The z- and p- statistics should be interpreted cautiously however, as generalised linear mixed models can suffer from severe small sample biases where the effective sample size relates more to the higher levels of clustering than individual observations.

Parameters 'b' are the mean function beta parameters, parameters 'cov' are the covariance function parameters in the same order as '\$covariance\$parameters', and parameters 'd' are the estimated random effects.

**Value**

No return value, called for side effects.

---

progress_bar	<i>Generates a progress bar</i>
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**Description**

Prints a progress bar

**Usage**

```
progress_bar(i, n, len = 30)
```

**Arguments**

i                    integer. The current iteration.  
 n                    integer. The total number of iterations  
 len                    integer. Length of the progress a number of characters

**Value**

A character string

**Examples**

```
progress_bar(10, 100)
```

---

Quantile	<i>Family declaration to support quantile regression</i>
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---

**Description**

Skeleton list to declare a quantile regression model in a 'Model' object.

**Usage**

```
Quantile(link = "identity", scaled = FALSE, q = 0.5)
```

**Arguments**

link	Name of the link function - any of 'identity', 'log', 'logit', 'inverse', or 'probit'
scaled	Logical indicating whether to include a scale parameter. If FALSE then the scale parameter is one.
q	Scalar in [0,1] declaring the quantile of interest.

**Value**

A list with two elements naming the family and link function

---

random.effects	<i>Extracts the random effect estimates</i>
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---

**Description**

Extracts the random effect estimates or samples from an mcml object returned from call of 'MCML' or 'LA' in the [Model](#) class.

**Usage**

```
random.effects(object)
```

**Arguments**

object	An 'mcml' model fit.
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**Value**

A matrix of dimension (number of fixed effects ) x (number of MCMC samples). For Laplace approximation, the number of "samples" equals one.

---

residuals.mcml	<i>Residuals method for a 'mcml' object</i>
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**Description**

Calling residuals on an 'mcml' object directly is not recommended. This function will currently only generate marginal residuals. It will generate a new 'Model' object internally, thus copying all the data, which is not ideal for larger models. The preferred method is to call residuals on either the 'Model' object or using 'Model\$residuals()', both of which will also generate conditional residuals.

**Usage**

```
## S3 method for class 'mcml'
residuals(object, type, ...)
```

**Arguments**

object	A 'mcml' object.
type	Either "standardized", "raw" or "pearson"
...	Further arguments passed from other methods

**Value**

A matrix with either one column is conditional is false, or with number of columns corresponding to the number of MCMC samples.

---

residuals.Model	<i>Extract residuals from a 'Model' object</i>
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**Description**

Return the residuals from a 'Model' object. This function is a wrapper for 'Model\$residuals()'. Generates one of several types of residual for the model. If conditional = TRUE then the residuals include the random effects, otherwise only the fixed effects are included. For type, there are raw, pearson, and standardized residuals. For conditional residuals a matrix is returned with each column corresponding to a sample of the random effects.

**Usage**

```
## S3 method for class 'Model'
residuals(object, type, conditional, ...)
```

**Arguments**

object	A 'Model' object.
type	Either "standardized", "raw" or "pearson"
conditional	Logical indicating whether to condition on the random effects (TRUE) or not (FALSE)
...	Further arguments passed from other methods

**Value**

A matrix with either one column is conditional is false, or with number of columns corresponding to the number of MCMC samples.

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setParallel	<i>Disable or enable parallelised computing</i>
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**Description**

By default, the package will use multithreading for many calculations if OpenMP is available on the system. For multi-user systems this may not be desired, so parallel execution can be disabled with this function.

**Usage**

```
setParallel(parallel_, cores_ = 2L)
```

**Arguments**

parallel_	Logical indicating whether to use parallel computation (TRUE) or disable it (FALSE)
cores_	Number of cores for parallel execution

**Value**

None, called for effects



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summary.mcml	<i>Summarises an mcml fit output</i>
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**Description**

Summary method for class "'mcml'"

**Usage**

```
## S3 method for class 'mcml'
summary(object, ...)
```

**Arguments**

object	an object of class "'mcml'" as a result of a call to MCML, see <a href="#">Model</a>
...	Further arguments passed from other methods

**Details**

'print.mcml' tries to replicate the output of other regression functions, such as 'lm' and 'lmer' reporting parameters, standard errors, and z- and p- statistics. The z- and p- statistics should be interpreted cautiously however, as generalised linear mixed models can suffer from severe small sample biases where the effective sample size relates more to the higher levels of clustering than individual observations.

Parameters 'b' are the mean function beta parameters, parameters 'cov' are the covariance function parameters in the same order as '\$covariance\$parameters', and parameters 'd' are the estimated random effects.

**Value**

A list with random effect names and a data frame with random effect mean and credible intervals

---

summary.Model	<i>Summarizes a 'Model' object</i>
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**Description**

Summarizes 'Model' object.

**Usage**

```
## S3 method for class 'Model'
summary(object, max_n = 10, ...)
```

**Arguments**

object	An 'Model' object.
max_n	Integer. The maximum number of rows to print.
...	Further arguments passed from other methods

**Value**

An object of class 'logLik'. If both 'fixed' and 'covariance' are FALSE then it returns NA.

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vcov.mcml	<i>Extract the Variance-Covariance matrix for a 'mcml' object</i>
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---

**Description**

Returns the calculated variance-covariance matrix for a 'mcml' object. The generating Model object has several methods to calculate the variance-covariance matrix. For the standard GLS information matrix see 'Model\$information\_matrix()'. Small sample corrections can be accessed directly from the generating Model using 'Model\$small\_sample\_correction()'. The variance-covariance matrix including the random effects can be accessed using 'Model\$information\_matrix(include.re = TRUE)'.

**Usage**

```
## S3 method for class 'mcml'
vcov(object, ...)
```

**Arguments**

object	A 'mcml' object.
...	Further arguments passed from other methods

**Value**

A variance-covariance matrix.

---

vcov.Model	<i>Calculate Variance-Covariance matrix for a 'Model' object</i>
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---

**Description**

Returns the variance-covariance matrix for a 'Model' object. Specifically, this function will return the inverse GLS information matrix for the fixed effect parameters. Small sample corrections can be accessed directly from the Model using 'Model\$small\_sample\_correction()'. The variance-covariance matrix including the random effects can be accessed using 'Model\$information\_matrix(include.re = TRUE)'.

**Usage**

```
## S3 method for class 'Model'
vcov(object, ...)
```

**Arguments**

object	A 'Model' object.
...	Further arguments passed from other methods

**Value**

A variance-covariance matrix.

---

yexample312a	<i>Data for first example in Section 3.12 of JSS paper</i>
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**Description**

Data for first example in Section 3.12 of JSS paper

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yexample312b	<i>Data for second example in Section 3.12 of JSS paper</i>
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**Description**

Data for second example in Section 3.12 of JSS paper

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yexample312c

*Data for third example in Section 3.12 of JSS paper*

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**Description**

Data for third example in Section 3.12 of JSS paper

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ytest1

*Data for model tests*

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**Description**

Data for model tests

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