

Package ‘corMLPE’

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Title Correlation Structures for Symmetric Relational Data

Version 0.1.0

Description Implements correlation structures for symmetric relational data (e.g. pairwise distances and dissimilarities) that interface with models using 'nlme'-style correlation structures. The maximum likelihood population effects method is described by Clarke et al. (2002) <doi:10.1198/108571102320>.

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corMaternMLPE

Correlation Structure for Grouped Matern MLPE Models

Description

Correlation Structure for Grouped Matern MLPE Models

Usage

```
corMaternMLPE(
  value = c(0.1, 0.1),
  nu = 2,
  form = ~1,
  distances = FALSE,
  fixed = FALSE
)
```

```
## S3 method for class 'corMaternMLPE'
as.matrix(x, ...)
```

Arguments

value	Numeric vector of length 2 with starting values 'c(stddev, range)'.
nu	Smoothness parameter for the Matern covariance kernel.
form	Formula identifying pair-members and optional grouping.
distances	A named list of distance matrices, one per group.
fixed	Logical; if 'TRUE', keep the correlation parameters fixed.
x	A fitted 'corMaternMLPE' correlation structure object.
...	Unused.

Value

A 'corStruct' object of class 'corMaternMLPE'.

corMLPE

*Correlation structure for symmetric relational data***Description**

Correlation structure for symmetric relational data

Coerce a 'corMLPE' Object to a Correlation Matrix

Usage

```
corMLPE(value = 0.1, form = ~1, fixed = FALSE)
```

```
## S3 method for class 'corMLPE'
as.matrix(x, ...)
```

Arguments

value	Starting value for the correlation parameter
form	A formula including two variables that give the unordered pair of elements associated with each observation, and optionally a grouping factor that indicates the set to which the elements belong. See 'Details'.
fixed	Optional. Logical, fit model with the starting value for the correlation parameter fixed
x	A fitted 'corMLPE' correlation structure object.
...	Unused.

Details

"Maximum likelihood population effects" (MLPE) is a correlation structure for dyadic, symmetric relational data: where each observation is a measurement for an unordered pair of elements from a set. For two (different) elements i, j , let $E[y_{i,j}]$ be the expectation of the response variable (perhaps conditional on some random effects), and

$$y_{i,j} = E[y_{i,j}] + \alpha_i + \alpha_j + \epsilon_{i,j},$$

where α are associated with unique elements of the set and are i.i.d zero-mean Gaussian random variables with standard deviation τ ; and ϵ are i.i.d Gaussian errors with standard deviation σ . Marginally (after integrating out α), the covariance between two observations $y_{i,j}$ and $y_{k,l}$ is

$$\text{cov}(y_{i,j}, y_{k,l}) = \tau^2(\delta(i, k) + \delta(j, l))$$

where the function δ evaluates to 1 when its arguments are equal and zero otherwise, and we order the indices so that $i < j, k < l$ for convenience.

The marginal variance is $\text{var}(y_{i,j}) = 2\tau^2 + \sigma^2$. The corresponding correlation structure has a single parameter, $\rho = \tau^2/(2\tau^2 + \sigma^2)$ which is constrained to lie between 0 and 0.5.

The "form" argument of a corMLPE object must contain two variables that indicate the pair of elements associated with each observation, and can optionally contain a grouping factor that indicates the set to which the elements belong. Elements from different sets are treated as distinct even if they have the same label, and thus there is always a zero correlation between measurements across different sets.

For example, if "data.frame(elem1 = c(1,1,2), elem2 = c(2,3,4), grp = c(1,1,2))" were used as data with "form=~elem1 + elem2 | grp", then the first two observations would be correlated (because they are from the same group and share the element "1"), but would both be uncorrelated with the third observation (as the third observation is associated with the second set, despite involving an element "2" that is labelled identically to an element from the first set). The ordering within a pair does not matter. Multiple observations of the same pair of elements are allowed, as are missing combinations of pairs, but "self" comparisons are not (where both elements of a pair are the same).

It is important to note that this correlation structure does not directly incorporate a (dis)similarity metric (which could instead be included as a covariate in the regression model), but instead tries to account for the dependence between pairwise measurements taken between the same objects.

Value

'corMLPE()' returns an object of class 'corMLPE' and 'corStruct' for use as a correlation structure in 'nlme::gls()' or 'nlme::lme()'. The object stores the MLPE correlation parameter and the formula that identifies the two members of each pairwise observation. The 'as.matrix()' method returns the implied observation-level correlation matrix for an initialized 'corMLPE' object.

References

Clarke et al. 2002. Confidence limits for regression relationships between distance matrices: estimating gene flow with distance. *Journal of Agricultural, Biological, and Environmental Statistics* 7: 361-372.

Examples

```
dat <- simulate_IBD_corMLPE(sets = 1, elements = 5, seed = 1)
fit <- nlme::gls(
  y ~ x,
  data = dat,
  correlation = corMLPE(form = ~pop1 + pop2)
)
coef(fit$modelStruct$corStruct, unconstrained = FALSE)
```

corNMLPE

Correlation Structure for Clustered NMLPE Models

Description

Correlation Structure for Clustered NMLPE Models

Usage

```
corNMLPE(
  value = c(0.1, 0.1, 0.1, 0.1, 0.1),
  nu = 2,
  form = ~1,
  clusters = FALSE,
  distances = FALSE,
  fixed = FALSE
)

## S3 method for class 'corNMLPE'
as.matrix(x, ...)
```

Arguments

value	Numeric vector of length 5 with starting values.
nu	Smoothness parameter for the Matern covariance kernel.
form	Formula identifying pair-members and optional grouping.
clusters	Named list (or vector for one group) of cluster IDs.
distances	Named list of distance matrices among clusters.
fixed	Logical; if 'TRUE', keep the correlation parameters fixed.
x	A fitted 'corNMLPE' correlation structure object.
...	Unused.

Value

A 'corStruct' object of class 'corNMLPE'.

corNMLPE2

Correlation Structure for Reduced-Basis NMLPE Models

Description

Correlation Structure for Reduced-Basis NMLPE Models

Usage

```
corNMLPE2(value = c(0.1, 0.1), form = ~1, clusters = FALSE, fixed = FALSE)

## S3 method for class 'corNMLPE2'
as.matrix(x, ...)
```

Arguments

value	Numeric vector of length 2 with starting values.
form	Formula identifying pair-members and optional grouping.
clusters	Named list (or vector for one group) of cluster IDs.
fixed	Logical; if 'TRUE', keep the correlation parameters fixed.
x	A fitted 'corNMLPE2' correlation structure object.
...	Unused.

Value

A 'corStruct' object of class 'corNMLPE2'.

dgCMatrix_corMLPE-methods

Methods for Internal 'dgCMatrix_corMLPE' Objects

Description

These methods preserve class identity required for 'mgcv::gamm()' compatibility when sparse matrix operations are applied.

Usage

```
## S4 method for signature 'dgCMatrix_corMLPE'
t(x)

## S4 method for signature 'dgCMatrix_corMLPE,index,missing,logical'
x[i, j, ..., drop = TRUE]

## S4 method for signature 'dgCMatrix_corMLPE,missing,index,logical'
x[i, j, ..., drop = TRUE]
```

Arguments

x	A 'dgCMatrix_corMLPE' object.
i	Row index.
j	Column index.
...	Additional arguments passed to matrix subsetting.
drop	Logical; passed to '[' methods.

Value

The 't()' method returns a transposed 'dgCMatrix_corMLPE' object. The '[' methods return row- or column-subsets while preserving the 'dgCMatrix_corMLPE' class. These methods are used internally so sparse matrices generated by 'corMLPE' remain compatible with downstream model fitting code.

Examples

```
m <- Matrix::sparseMatrix(i = c(1, 2), j = c(1, 2), x = 1)
m <- methods::as(m, "dgCMatix_corMLPE")
class(t(m))
class(m[1, , drop = FALSE])
```

`simulate_corMLPE_residuals`*Simulate data from a fitted corMLPE model*

Description

Simulate data from a fitted corMLPE model

Usage

```
simulate_corMLPE_residuals(model, n = 1, seed = NULL)
```

Arguments

model	fitted model of class 'gls' with corMLPE correlation structure
n	number of simulations
seed	random seed

Value

A numeric matrix with one row per observation in 'model' and one column per simulation. Values are simulated residual vectors with the fitted 'corMLPE' dependence structure and the fitted residual standard deviation from the 'gls' model.

Examples

```
dat <- simulate_IBD_corMLPE(sets = 1, elements = 5, seed = 1)
fit <- nlme::gls(
  y ~ x,
  data = dat,
  correlation = corMLPE(form = ~pop1 + pop2)
)
sims <- simulate_corMLPE_residuals(fit, n = 2, seed = 2)
dim(sims)
```

simulate_IBD_corMLPE *Simulate data from an isolation-by-distance model with MLPE correlation structure*

Description

Simulate data from an isolation-by-distance model with MLPE correlation structure

Usage

```
simulate_IBD_corMLPE(
  sets = 1,
  elements = rep(10, sets),
  intercept = 0,
  slope = 0.5,
  random_effects = diag(2),
  correlation = 0.25,
  residual_sd = 1,
  distances = NULL,
  seed = 1
)
```

Arguments

sets	number of distinct sets (e.g. species) containing elements that are compared
elements	vector, number of elements (e.g. populations, individuals) in each set
intercept	intercept of regression line
slope	slope of regression line
random_effects	variance-covariance matrix for random intercepts/slopes per set; ignored if sets==1
correlation	parameter of MLPE correlation structure; between 0 and 0.5
residual_sd	standard deviation of (correlated) errors
distances	optional; list of distance matrices (one for each set), or a single distance matrix if sets==1; if absent, locations are simulated from a 2d uniform distribution
seed	random seed used to simulate data

Value

A data frame with one row per pairwise observation and columns 'y', 'pop1', 'pop2', 'set', and 'x'. The response 'y' is simulated from an isolation-by-distance model with MLPE-correlated errors, 'pop1' and 'pop2' identify the paired elements, 'set' identifies the group, and 'x' is the pairwise distance. Model settings and simulated random effects are stored as attributes.

Examples

```
dat <- simulate_IBD_corMLPE(sets = 1, elements = 5, seed = 1)
head(dat)
attr(dat, "correlation")
```

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