# Package 'multivator'

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Type Package

**Version** 1.1-10

Title A Multivariate Emulator

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Suggests abind
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<b>Description</b> A multivariate generalization of the emulator package.
License GPL-2
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R topics documented:
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# Description

A generalization of the emulator as discussed in Hankin 2005

#### **Details**

Package: multivator
Type: Package
Version: 1.0
Date: 2009-10-27
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LazyLoad: yes

## Author(s)

Robin K. S. Hankin

Maintainer: <hankin.robin@gmail.com>

#### References

R. K. S. Hankin 2005. "Introducing BACCO, an R bundle for Bayesian Analysis of Computer Code Output". *Journal of Statistical Software*, 14(16).

R. K. S. Hankin (2012). "Introducing multivator: A Multivariate Emulator"  $Journal\ of\ Statistical\ Software,\ 46(8),\ 1-20.\ doi:\ 10.18637/jss.v046.i08$ 

#### See Also

multem

```
data(mtoys)
d <- obs_maker(toy_mm, toy_mhp, toy_LoF, toy_beta)
ex <- experiment(toy_mm,d)
multem(toy_mm2, ex, toy_mhp, toy_LoF,give=TRUE)</pre>
```

apart 3

apart

Decompose a matrix with multiple columns of dependent variables

#### **Description**

Decomposes a matrix with multiple columns of dependent variables into a mdm object

# Usage

```
apart(X, dependent, use_rownames = TRUE)
```

## **Arguments**

X A matrix with columns corresponding to either independent variables or de-

pendent variables. The names of the independent variables are taken from the

column names of X

dependent Vector of length ncol(X). If numeric, interpret as the column numbers of the

dependent variable. If logical, TRUE elements correspond to dependent variables

use\_rownames Boolean, with default TRUE meaning to use the rownames of X to create row-

names in the returned value

#### Value

Returns an object of class experiment.

#### Author(s)

Robin K. S. Hankin

## See Also

```
as.list
```

```
data(e3mg)
apart(e3mg , 6:7)

a <- round(emulator::latin.hypercube(6,5),2)
rownames(a) <- c("first", "second", "third", "fourth", "fifth", "sixth")
colnames(a) <- c(letters[1:3], "length", "depth")
jj_expt <- apart(a,4:5)  # use of apart()

x <- get_mdm(jj_expt[c(1,7)])
xold(x) <- 0.5

multem(x,jj_expt,hp=as.mhp(x),give=TRUE)</pre>
```

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as.separate

Split an object of class experiment into a list of univariate datasets

## **Description**

Split an experiment object into univariate designs; return a list with elements suitable for univariate analysis with the emulator package.

# Usage

```
as.separate(expt)
```

## **Arguments**

expt

Object of class experiment

## Author(s)

Robin K. S. Hankin

# **Examples**

```
require(emulator)

data(mtoys)
d <- obs_maker(toy_mm, toy_mhp, toy_LoF, toy_beta)

ex <- experiment(toy_mm, d)
jj <- as.separate(ex)  #list of 3: temp,rain,humidity

# now use it in a univariate emulator:
kk <- jj$temp
interpolant.quick(x=latin.hypercube(3,4),d=kk$obs,xold=kk$val,scales=rep(1,4))</pre>
```

betahat

Various intermediate expressions needed by the multivariate emulator

# Description

Various intermediate expressions needed by the multivariate emulator

betahat 5

#### Usage

```
regressor(x,LoF)
beta_hat(expt,hp,LoF, ...)
betahat_mult(H, Sigmainv, d)
betahat_mult_Sigma(H, Sigma, d)
cstar(x1, x2=x1, expt, hp, LoF = NULL, Sigmainv=NULL, ...)
eq2.36(H, Sigmainv, d, log=TRUE)
eq2.36_Sigma(H, Sigma, d)
var.matrix(x1,x2=x1,hp, ...)
```

#### **Arguments**

x,x1,x2	Objects of class mdm: multivariate design matrix
Н	Matrix of regressors (create this with regressor())
d	Vector of observations, possibly not all of the same dimensions (eg some elements might be Kelvin, others millimeters of rain per year)
expt	Object of class experiment
Sigma	The variance matrix of d
log	Boolean, with TRUE meaning to return the logarithm of the answer
Sigmainv	The inverse of the variance matrix of d, with default NULL meaning to calculate it directly using $var.matrix()$
LoF	A list of functions with default NULL meaning to use default_LoF()
hp	Object of class mhp: multivariate hyperparameters
	Extra arguments which are passed (via var.matrix()) to corr.matrix() of the emulator package

#### **Details**

Function regressor() creates a (sort of) direct sum of regressor matrices for an overall regressor matrix. It returns a matrix whose rows are the regressor functions for each row in the df argument. Each type of observation has its own 'slot' of columns, the others being filled with zeros.

The emulator package *should* have used this method (rather than messing about with regressor.basis() and regressor.multi()).

To get the regression coefficients, the user should use function beta\_hat(), which is the user-friendly version. It is a wrapper for function betahat\_mult\_Sigma().

The equation for var.matrix() is

$$c^*\left(x,x'\right) = c\left(x,x'\right) - t(x)^TA^{-1}t(x') + \left\{h(x)^T - t(x)^TA^{-1}H\right\} \left(H^TA^{-1}H\right)^{-1} \left\{h(x')^T - t(x')^TA^{-1}H\right\}^T$$

## Author(s)

Robin K. S. Hankin

## See Also

multem

6 compatible

#### **Examples**

```
data(mtoys)

H <- regressor(toy_mm, toy_LoF)
Sigma <- var.matrix(toy_mm, hp=toy_mhp)
Sigmainv <- solve(Sigma)

jj <- toy_mm_maker(34,35,36)
expt <- experiment(jj,obs_maker(jj,toy_mhp,toy_LoF,toy_beta))

x1 <- jj[c(20,40,100),]
xold(x1) <- 0.2

x2 <- jj[c(11,21:24,40:42),]
xold(x2) <- xold(x2)+0.1

#primary function of package:
multem(x=x1, expt, hp=toy_mhp, LoF=toy_LoF)

# conditional covariance matrix:
cstar(x1,x2, expt, hp=toy_mhp, LoF=toy_LoF)</pre>
```

compatible

Are two objects compatible?

## **Description**

Function to detect whether two objects are compatible

# Usage

```
compatible(x1,x2)
```

## **Arguments**

x1,x2

Two objects with names and levels. Typically either objects of class mhp or mdm.

#### **Details**

Here, "compatible" means have the same names and levels. If an mdm object and mhp object are compatible, then they may be supplied to (eg) var.matrix().

The function uses identical() to compare the names and levels.

## Value

Returns a Boolean.

#### Note

Cannot yet compare LoF objects.

default\_LoF 7

#### Author(s)

Robin K. S. Hankin

# **Examples**

```
data(mtoys)
stopifnot(compatible(toy_mhp, toy_mm))
```

default\_LoF

Default List of functions

# Description

Creates a default List of Functions for use with regressor().

# Usage

```
default_LoF(x)
```

# **Arguments**

Х

Object with names and levels methods; typically of class mdm or mhp.

# Value

Returns a named list with each element giving the regressor functions for that level.

## Author(s)

Robin K. S. Hankin

## See Also

regressor

```
data(mtoys)

default_LoF(toy_mm) # note list names == levels(toy_mm)

regressor(toy_mm) # use default
regressor(toy_mm , toy_LoF) # use a bespoke set
```

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e3mg

Output from computer model e3mg

#### **Description**

Output from computer model e3mg detailing the depth of the recession and its length as a function of four exogenous parameters

## Usage

```
data(e3mg)
```

#### **Format**

- e3mg is a matrix with 843 rows and 6 columns. Four of the columns are exogenous variables (oil.price, direct.tax, interest.rate, and saving.ratio) and two are model outputs: rec\_len, the length (in years) of the recession, and dep\_rec, the depth of the recession.
- e3mg\_LoF is a list of functions suitable for use with the e3mg dataset

#### **Details**

The data comprises 843 runs of the e3mg econometric model, used to predict the recession precipitated by the banking crisis.

The depth of the recession is defined as the maximum difference between predicted post-crash GDP and GDP immediately pre-crash.

The length of the recession is defined as the time in years required for GDP to return to pre-crash levels.

#### **Source**

Data kindly provided by Cambridge Econometrics

#### See Also

apart

```
data(e3mg)
a <- lm(rec_len~oil.price*direct.tax + direct.tax*saving.ratio + investment,data=data.frame(e3mg))
b <- lm(rec_dep~oil.price*direct.tax + direct.tax*saving.ratio + investment,data=data.frame(e3mg))
plot(residuals(a),residuals(b))  # correlated!

# define an experiment object and find optimal prarams
e3mg_expt <- apart(e3mg[1:20,],6:7)
opt <- optimal_params(e3mg_expt, e3mg_LoF, option='c')

# now a point in parameter space:
center <- get_mdm(e3mg_expt)[c(1,40),]</pre>
```

experiment 9

```
rownames(center) <- c('center_dep','center_len')
xold(center) <- 0
#now predict the behaviour at the center:
multem(center, e3mg_expt, hp=opt, e3mg_LoF, give = TRUE)</pre>
```

experiment

Multivatriate hyperparameter (mhp) objects

## **Description**

Create and manipulate multivariate hyperparameter (mhp) objects

## Usage

```
experiment(mm,obs)
```

#### **Arguments**

mm Object of class mdm

obs Vector of observations, with elements corresponding to the rows of mm

#### **Details**

An "experiment" is an ordered pair of a multivariate design matrix and a vector of observations with entries corresponding to the rows of the design matrix.

It functions as a container for the design matrix and observations. It is intended to simplify the calls to many functions in the package which require a design matrix and vector of observations.

There are two get methods, get\_mdm() and get\_obs(), for the design matrix and observations respectively. Note the deliberate absence of set methods.

#### Value

Returns an object of class experiment, which is used as input to many of the functions in the package.

## Author(s)

Robin K. S. Hankin

```
data(mtoys)
jj_expt <- experiment(toy_mm,toy_d)

# accessor methods:
get_obs(jj_expt)
get_mdm(jj_expt)</pre>
```

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```
# estimation of coefficients:
beta_hat(jj_expt, toy_mhp, toy_LoF)

# use multem():
multem(toy_mm3, jj_expt, toy_mhp, toy_LoF,give=TRUE)
```

head

Head and tail

# Description

Print the first few, or last few, lines of a mdm object

# Usage

```
## S4 method for signature 'mdm' head(x, n = 6, ...)
## S4 method for signature 'mdm' tail(x, n = 6, ...)
```

# **Arguments**

```
x object of class mdmn number of lines to print as per same argument in head() and tail()... Further arguments passed to head() or tail()
```

## Value

Returns a truncated mdm object. The levels of the types are unchanged.

# Author(s)

Robin K. S. Hankin

```
data("mtoys")
head(toy_mm)
tail(toy_mm,3)
```

ipd 11

ipd

Positive definite matrices

## **Description**

Is a matrix symmetric positive-definite?

#### Usage

```
ipd(mat)
```

#### **Arguments**

mat

A matrix

#### Value

Returns either TRUE if symmetric positive-definite; or FALSE, printing a diagnostic message.

#### Author(s)

Robin K. S. Hankin

# **Examples**

```
data(mtoys)
stopifnot(ipd(crossprod(matrix(rnorm(30),10))))
stopifnot(ipd(M(toy_mhp)))
```

mcneal1

Dataset due to McNeall

# **Description**

Data, due to McNeall, from 92 runs of a climate model

## Usage

```
data(mcneall)
```

#### **Details**

McNeall used a numerical climate model and ran it 92 times, on a design matrix specified on 16 independent variables as detailed in McNeall 2008.

The model output is a temperature distribution over the surface of the Earth. The model gives 2048 temperatures, corresponding to 2048 grid squares distributed over the Earth. A vector of 2048 temperatures may be displayed on a global map using the showmap() function.

The 92 model runs are presented in the form of a 2048 by 92 matrix mcneal1\_temps, each column of which corresponds to a run. A row of 92 temperatures corresponds to the temperature at a particular place on the earth as predicted by each of the 92 model runs.

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Following McNeall, a principal component analysis on the maps was performed. The first four were used. Matrix eigenmaps is a 2048 by 4 matrix, with columns corresponding to the four principal components.

Matrix mcneal1\_pc is a 92-by-20 matrix. The first 16 columns correspond to the independent variables (ie the design matrix); columns 17-20 correspond to the first four principal components of the model output. The 92 rows correspond to the 92 model runs.

The package can be used on the mcneall\_temps matrix; use apart() to generate a mdm object. A reasonably optimized hyperparameters object of class mhp is given as opt\_mcneall.

#### References

D. McNeall 2008. "Dimension Reduction in the Bayesian analysis of a numerical climate model". PhD thesis, University of Southampton.

#### See Also

```
showmap
```

## **Examples**

```
data(mcneall)
showmap(mcneall_temps[,1], pc=FALSE,landmask=landmask)
```

mdm

Multivariate design matrices

## **Description**

Multivariate design matrices are represented using objects of class mdm.

## Usage

```
mdm(xold, types)
as.mdm(x, ...)
is.mdm(x)
as.list(x, ...)
as.matrix(x, ...)
## S4 method for signature 'mdm,missing,missing'
as.data.frame(x, row.names=NULL,optional=TRUE, ...)
## S4 method for signature 'mdm'
rbind(x, ..., deparse.level=1)
types(x)
xold(x)
```

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## **Arguments**

xold Matrix of design points, each row being a point in parameter space
types A factor holding the types of each observation

x An object of class mdm
row.names,optional
Currently ignored
... Further arguments passed to NextMethod()

deparse.level As for rbind()

## **Details**

Various functionality for creating and manipulating objects of class mdm (Multivariate Design Matrix).

## Note

The internal representation has two slots, one for the design matrix proper (a matrix), and one for the types of observation (a factor).

## Author(s)

Robin K. S. Hankin

#### See Also

```
mhp,apart
```

## **Examples**

```
mm <- toy_mm_maker(7,8,9)
is.mdm(mm)
xold(mm) <- matrix(rnorm(108),27,4)
mm[1,1] <- 0.3
data(mtoys)
obs_maker(mm,toy_mhp,toy_LoF,toy_beta)</pre>
```

mhp

Multivatriate hyperparameter (mhp) objects

# Description

Create and manipulate multivatriate hyperparameter (mhp) objects

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#### Usage

```
mhp(M, B, levels = NULL, names = NULL)
is.mhp(x)
M(x)
M(x) <- value
B(x)
B(x) <- value
levels(x)
summary(object,...)</pre>
```

# **Arguments**

М	Variance matrix (must be positive definite)
В	Array of roughness parameters. Each slice (ie B[,,i]) must be positive-definite
levels	Character vector holding the levels. Default NULL means to use rownames (M) or dimnames (B[[3]])
names	Character vector holding the names of the dimensions. Default of NULL means to use $dimnames(B[[1]])$
x,object	Object of class mhp
value	Replacement object
	Further arguments passed to the summary method

## **Details**

An mhp object *must* have names and levels, so either provide them explicitly with the eponymous arguments, or give named arrays to M and B.

# Value

Returns an object of class mhp

## Author(s)

Robin K. S. Hankin

## See Also

 $\mathsf{mdm}$ 

```
hp <- mhp(M=diag(2),B=array(c(diag(3),diag(3)),c(3,3,2)),
names=letters[1:3],levels=c("oak","ash"))
M(hp)
B(hp)[1,1,1] <- 30  # try a negative value and see what happens
names(hp)
names(hp) <- c("Alice","Zachy","Annabel")
levels(hp) <- c("squid","snail")
summary(hp)</pre>
```

mtoys 15

mtoys

Toy datasets

# Description

Toy datasets that illustrate the package

#### Usage

```
toy_LoF
toy_mm
toy_mm2
toy_mm3
toy_mhp
```

#### **Format**

- toy\_LoF is a list of three functions that work with regressor() and toy\_df
- toy\_M is an example M matrix for use with mhp()
- toy\_B is an example of a B array of roughness coefficients for use with mhp()
- toy\_mm and toy\_mm2 are examples of a mdm object, generated with function toy\_mm\_maker(). These objects are marginals from the *same* multivariate observation.
- toy\_mm3 and toy\_mm4 are small examples of mdm objects
- toy\_mhp is an example of a mhp object
- toy\_beta is a numeric vector that works with the above objects

#### **Details**

These objects are intended as simple working 'toy' examples of the various things needed to use the emulator.

Note that toy\_d and toy\_d2 are the marginals of the *same* observation (see the vignette).

#### Author(s)

Robin K. S. Hankin

## References

• R. K. S. Hankin 2005. *Introducing BACCO, an R bundle for Bayesian analysis of computer code output,* Journal of Statistical Software, 14(16)

## See Also

```
toy_mm_maker
```

16 multem

## **Examples**

```
data(mtoys)
obs_maker(toy_mm, toy_mhp, toy_LoF, toy_beta)
multem(toy_mm2,toy_expt,toy_mhp,toy_LoF,give=TRUE)
```

multem

The multivariate emulator

# Description

A multivariate generalization of the interpolant() function of the emulator package

# Usage

```
multem(x, expt, hp, LoF = NULL, give=FALSE, Sigmainv=NULL, ...)
```

# Arguments

X	Points at which the function is to be estimated in the form of an object of class mdm
expt	Points at which the code has been evaluated (x $_{\rm known}$ ), in the form of an object of class experiment
hp	hyperparameter object, of class mhp
give	Boolean, with TRUE meaning to return extra information and default FALSE meaning to return just the mean $$
Sigmainv	The inverse of the variance matrix of the observations with default NULL meaning to calculate using ${\tt var.matrix}()$
LoF	List of regressor functions
	Further arguments passed to var.matrix()

#### **Details**

This is the central function of the package. It is the analogue of interpolant() of the emulator package.

# Author(s)

Robin K. S. Hankin

# See Also

```
betahat_mult
```

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## **Examples**

```
data(mtoys)
d <- obs_maker(toy_mm, toy_mhp, toy_LoF, toy_beta)
ex <- experiment(toy_mm , d)

Sigmainv <- solve(var.matrix(toy_mm,hp=toy_mhp))
multem(x=toy_mm2, expt=ex, hp=toy_mhp,LoF=toy_LoF, give=TRUE)</pre>
```

obs\_maker

Create observations

# Description

A function to create observations using known parameters and hyperparameters

# Usage

```
obs_maker(x, hp, LoF, beta, Sigma=NULL, ...)
```

## **Arguments**

X	Object of class mdm: each row is a point in parameter space
hp	Object of class mhp
LoF	List of functions
beta	Vector of regression coefficients
Sigma	Variance matrix, with default NULL meaning to use $var.matrix(x,hp)$
	Further arguments passed to var.matrix()

#### **Details**

Uses the mytnorm package to generate observations directly from the parameters and hyperparameters as a Gaussian process.

## Value

Returns a (named) vector of observations. Note that the observations may have different units (eg temperature in Kelvin, rainfall in millimeters per year).

## Author(s)

Robin K. S. Hankin

## See Also

```
toy_mm_maker
```

18 optimal\_params

#### **Examples**

```
data(mtoys)
d <- obs_maker(toy_mm , toy_mhp, toy_LoF, toy_beta)
d <- obs_maker(toy_mm_maker(6,7,8) , toy_mhp, toy_LoF, toy_beta)</pre>
```

optimal\_params

Optimization of the hyperparameters

## **Description**

Optimization of the hyperparameters using a sequence of subfunctions.

#### Usage

```
optimal_params (expt, LoF, start_hp, option = "a", ...)
optimal_B (expt, LoF, start_hp, option = "a", verbose=FALSE, ...)
optimal_identical_B(expt, LoF, start_hp, verbose=FALSE, ...)
optimal_diag_M (expt, LoF, start_hp)
optimal_M (expt, LoF, start_hp, ...)
```

#### **Arguments**

expt	Object of class experiment
LoF	List of functions
start_hp	Start value for the hyperparameters, an object of class mhp. The various optimization routines use the different parts of start_hp as start points, and incrementally update it
option	In function optimal_B() and consequently optimal_params(), a character indicating whether to allow the scales to differ or not.
	<ul> <li>Default option "a" is the simplest: each univariate B matrix is a multiple of the identity matrix.</li> <li>Option "b" allows the B matrices to be any (positive definite) diagonal matrix.</li> </ul>
	<ul> <li>Option "c" specifies that B[,,j] is diagonal for each j and furthermore that B[i,i,1]=B[i,i,2]==B[i,i,r]. This option calls optimal_identical_B().</li> </ul>
verbose	In function optimal_B(), Boolean with TRUE meaning to print debugging information and default FALSE meaning not to print anything
	Further arguments passed to the optimization routine

# **Details**

The user-friendly wrapper function is optimal\_params(). This calls function optimal\_B() first, as most of the analysis is conditional on B. Then optimal\_diag\_M() is called; this places the maximum likelihood estimate for  $\sigma^2$  on the diagonal of M. Finally, optimal\_M() is called, which assigns the off-diagonal elements of M.

Each of the subfunctions returns an object appropriate for insertion into a mhp object.

The "meat" of optimal\_params() is

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See how object out is modified sequentially, it being used as a start point for the next function.

#### Value

Returns a mhp object.

#### Note

Function optimal\_diag\_M() uses MLEs for the diagonals, but using each type of observation separately. It is conceivable that there is information that is not being used here.

## Author(s)

Robin K. S. Hankin

## **Examples**

```
data(mtoys)
optimal_params(toy_expt,toy_LoF,toy_mhp,option='c',control=list(maxit=1))
```

Print

Methods for printing mhp and mdm objects

## **Description**

Methods for printing nicely

## Usage

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

## **Arguments**

```
x An object of class mdm or mhp... Further arguments (currently ignored)
```

#### Author(s)

Robin K. S. Hankin

```
data(mtoys)
a <- as.mhp(toy_mm)
a</pre>
```

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showmap	Function to plot the McNeall dataset
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# Description

A small wrapper function to plot a global map of temperature, which is useful when analyzing the McNeall dataset

## Usage

```
showmap(z, pc, landmask, ...)
```

# Arguments

Z	A vector of length 2048 corresponding to temperatures on the Earth's surface
рс	Boolean, with TRUE meaning to interpret $z$ as a principal component and FALSE meaning to interpret $z$ as a temperature map
landmask	A matrix of zeros and ones corresponding to the Earth's surface with zero indicating sea and one indicating land; use data(mcneall)
	Further arguments passed to filled.contour()

# Author(s)

Robin K. S. Hankin

#### See Also

mcneal1

# **Examples**

```
data(mcneall)
showmap(mcneall_temps[,1],pc=FALSE,landmask=landmask)
```

ss

Overall variance matrix

# Description

Calculates the maximum correlations possible consistent with the roughness parameters

# Usage

```
ss(A, B, Ainv, Binv)
ss_matrix(hp,useM=TRUE)
ss_matrix_simple(hp,useM=TRUE)
```

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#### **Arguments**

A,B Positive-definite matrices (roughness parameters)

Ainv, Binv The inverses of A and B; if missing, compute explicitly

hp An object of class mhp

useM Boolean, with default TRUE meaning to multiply (pointwise) by M and FALSE

meaning not to (so giving the maximum correlation consistent with the rough-

ness matrices B)

#### **Details**

Function ss() calculates the maximum possible correlation between observations of two Gaussian processes at the same point (equation 24 of the vignette):

$$\left| \left( \frac{1}{2} B_r + \frac{1}{2} B_s \right) \left( \frac{1}{2} B_r^{-1} + \frac{1}{2} B_s^{-1} \right) \right|^{-1/4}$$

Functions ss\_matrix() and ss\_matrix\_simple() calculate the maximum covariances among the types of object specified in the hp argument, an object of class mhp. Function ss\_matrix() is the preferred form; function ss\_matrix\_simple() is a less efficient, but more transparent, version. The two functions should return identical output.

#### Value

Function ss() returns a scalar, ss\_matrix() a matrix of covariances.

#### Note

Thanks to Stephen Stretton for a crucial insight here

# Author(s)

Robin K. S. Hankin

#### **Examples**

```
data(mtoys)
ss_matrix(toy_mhp)
```

toy\_mm\_maker

Make a toy mm object

#### **Description**

Create a toy mhp object with three levels: temperature, rainfall, and humidity.

## Usage

```
toy_mm_maker(na, nb, nc, include_first = TRUE)
```

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# Arguments

na, nb, nc Numbers of observations for each level

include\_first Boolean, with default TRUE meaning to include an extra observation of each level

at the midpoint of the domain

# Value

Returns an object of class mhp.

# Author(s)

Robin K. S. Hankin

```
toy_mm_maker(4,5,6,FALSE)
toy_mm_maker(1,1,2,TRUE)
```

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