Package 'AHM'

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Type Package

Title Additive Heredity Model: Method for the Mixture-of-Mixtures Experiments

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Description An implementation of the additive heredity model for the mixture-of-mixtures experiments of Shen et al. (2019) in Technometrics <doi:10.1080/00401706.2019.1630010>. The additive heredity model considers an additive structure to inherently connect the major components with the minor components. The additive heredity model has a meaningful interpretation for the estimated model because of the hierarchical and heredity principles applied and the nonnegative garrote technique used for variable selection.

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Encoding UTF-8

LazyData true

Imports mixexp, plgp, devtools, dplyr, tibble, tidyr, Matrix

Depends R (>= 2.10), quadprog, glmnet

Suggests knitr, rmarkdown, partitions

VignetteBuilder knitr

BuildVignettes yes

RoxygenNote 6.0.1

NeedsCompilation no

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Description

This is one of the main functions. The function ahm computes the proposed additive heredity model.

Usage

```
ahm(y, x, num_major = 3, dist_minor = c(2, 2, 1), type = "weak",
   alpha = 0, lambda_seq = seq(0, 5, 0.01), nfolds = NULL,
   mapping_type = c("power"), powerh = 0, rep_gcv = 100)
```

Arguments

У	numeric vector
х	data.frame Note the column names of the x should be in the order of major components, minor components, and no interactions are needed.
num_major	number of major components
dist_minor	the allocation of number of minor components nested under major components
type	heredity type, weak heredity is the current support type
alpha	$0 is for the ridge in glmnet \ https://web.stanford.edu/~hastie/glmnet/glmnet_alpha.html\\$

check_col_correlation 3

lambda_seq a numeric vector for the options of lambda used in ridge regression for estimat-

ing the initials

nfolds used in cv.glmnet for initial value of parameters in the non-negative garrote

method

mapping_type the form of the coefficient function of major components in front of correspond-

ing minor terms. Currently only support "power"

powerh the power parameter used for the power function

rep_gcv the number of choices of tuning parameter used in the GCV selection

Value

Return a list

Examples

check_col_correlation Check column correlations

Description

Check column correlations

Usage

```
check_col_correlation(dat)
```

Arguments

data.frame

```
data("pringles_fat")
data_fat = pringles_fat
h_tmp = 1.3
x = data_fat[,c("c1","c2","c3","x11","x12","x21","x22")]
check_col_correlation (dat=x)
```

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coating

Photoresist-coating experiment data

Description

Photoresist-coating experiment data

Usage

```
data(coating)
```

Format

data.frame

References

Cornell, J.A. and Ramsey, P.J. (1998). A Generalized mixture model for categorized-components problems with an application to a photoresist-coating experiment. *Technometrics*, 40(1), 48-61. (tandfonline)

Examples

```
data(coating)
print(coating)
```

coef.ahm

Coefficient method for the fitted ahm object

Description

Coefficient method for the fitted ahm object

Usage

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

Arguments

```
object ahm object ... not used
```

Value

a numerical vector

coef.cv.ahm 5

Examples

coef.cv.ahm

Coefficient method for the fitted cv.ahm object

Description

Coefficient method for the fitted cv.ahm object

Usage

```
## S3 method for class 'cv.ahm'
coef(object, metric = "mse", ...)
```

Arguments

```
object cv.ahm object
metric "mse" or "aicc"
... not used
```

Value

a numerical vector

```
data("pringles_fat")
data_fat = pringles_fat
h_tmp = 1.3
x = data_fat[,c("c1","c2","c3","x11","x12","x21","x22")]
y = data_fat[,1]
powerh_path = round(seq(0.001,2,length.out =15),3)
num_major = 3; dist_minor = c(2,2,1)
res = cv.ahm (y, x, powerh_path=powerh_path, metric = "mse", num_major, dist_minor, type = "weak", alpha=0, lambda_seq=seq(0,5,0.01), nfolds=NULL, mapping_type = c("power"), rep_gcv=100)
coefficients = coef(res)
```

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compute AICc

Description

```
compute AICc
```

Usage

```
compute_aicc(rss, n, p, type = "AICc")
```

Arguments

rss	residual sum of squares
n	number of observation
p	number of nonzero parameters
type	character "AICc"

References

Calculating AIC "by hand" in R in Stack Overflow

Examples

```
compute_aicc (rss=10, n=30, p=6, type = "AICc")
```

cv.ahm

This is one of the main functions. It perform the cross validation on ahm models to select the optimal setting of hyper parameter h

Description

This is one of the main functions. It perform the cross validation on ahm models to select the optimal setting of hyper parameter h

Usage

```
cv.ahm(y, x, powerh_path = NULL, metric = c("mse", "AICc"), num_major = 3,
  dist_minor = c(2, 2, 1), type = "weak", alpha = 0, lambda_seq = seq(0,
  5, 0.01), nfolds = NULL, mapping_type = c("power"), rep_gcv = 100)
```

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Arguments

У	numeric vector
х	data.frame Note the column names of the x should be in the order of major components, minor components, and no interactions between major or minor components are needed.
powerh_path	if NULL, then the default is the vector: round(seq(0.001,2,length.out =15),3)
metric	"mse" or "AICc" the metric used in cross validtion where the minimum is selected as the optimal
num_major	number of major components
dist_minor	the allocation of number of minor components nested under major components
type	heredity type, weak heredity is the current support type
alpha	$0 is for the ridge in glmnet \ https://web.stanford.edu/~hastie/glmnet/glmnet_alpha.html\\$
lambda_seq	a numeric vector for the options of lambda used in ridge regression for estimating the initials
nfolds	used in cv.glmnet for initial value of parameters in the non-negative garrote method
mapping_type	the form of the coefficient function of major components in front of corresponding minor terms. Currently only support "power"
rep_gcv	the number of choices of tuning parameter used in the GCV selection

Value

Return a list

```
data("pringles_fat")
data_fat = pringles_fat
h_tmp = 1.3
x = data_fat[,c("c1","c2","c3","x11","x12","x21","x22")]
y = data_fat[,1]
powerh_path = round(seq(0.001,2,length.out =15),3)
num_major = 3; dist_minor = c(2,2,1)
res = cv.ahm (y, x, powerh_path=powerh_path, metric = "mse", num_major, dist_minor, type = "weak", alpha=0, lambda_seq=seq(0,5,0.01), nfolds=NULL, mapping_type = c("power"), rep_gcv=100)
object = res$metric_mse
```

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Description

Design points for the simplex centroid design with 3 components

Usage

```
data(design_simplex_centroid_design_3_major_component)
```

Format

data.frame

Examples

```
data(design_simplex_centroid_design_3_major_component)
print(design_simplex_centroid_design_3_major_component)
```

enlist

Create a list

Description

Create a list

Usage

```
enlist(...)
```

Arguments

... object to be included as elements in the list

```
item = c(1:10)
enlist(item)
```

expand_interactions 9

expand_interactions Expand the interaction terms for each subset group, say x11, x12, or c1, c2, c3

Description

Expand the interaction terms for each subset group, say x11, x12, or c1, c2, c3

Usage

```
expand_interactions(dat, sel_names)
```

Arguments

dat data frame sel_names characters

Examples

```
data("pringles_fat")
data_fat = pringles_fat
h_tmp = 1.3
x = data_fat[,c("c1","c2","c3","x11","x12","x21","x22")]
expand_interactions (dat=x, sel_names=c("c1", "c2", "c3"))
```

find_condition_num

Compute the conditional number of design matrix

Description

Compute the conditional number of design matrix

Usage

```
find_condition_num(x)
```

Arguments

(

matrix to be used in svd

```
data("pringles_fat")
data_fat = pringles_fat
h_tmp = 1.3
x = data_fat[,c("c1","c2","c3","x11","x12","x21","x22")]
find_condition_num (x)
```

10 mymaximin

mapping_function	Mapping_function is a function to add the functional coefficients of major components in front of minor components terms

Description

Mapping_function is a function to add the functional coefficients of major components in front of minor components terms

Usage

```
mapping_function(x, num_major = 3, dist_minor = C(2, 2, 1),
    mapping_type = c("power"), powerh = 0)
```

Arguments

x	data.frame Note the column names of the x should be in the order of major components, minor components, and no interactions are needed.
num majar	•
num_major	number of major components
dist_minor	the allocation of number of minor components nested under major components
mapping_type	the form of the coefficient function of major components in front of corresponding minor terms. Currently only support "power"
powerh	the power parameter used for the power function

Value

data frame

Examples

```
data("pringles_fat")
data_fat = pringles_fat
h_tmp = 1.3
x = data_fat[,c("c1","c2","c3","x11","x12","x21","x22")]
mapping_function(x=x, num_major=3, dist_minor=c(2,2,1), mapping_type = c("power"), powerh=0)
```

mymaximin The mymaximin function generates the matrix of maximin design points. It uses the simplex centroid design as the base design, then

in a stochastics way sample the candidate design points generated by

the function partition.

Description

This method is modified based on Prof. Bobby Gramacy's Computer Experiment lecture at Virginia Tech. Prof. Gramacy's lecture website

mymaximin 11

Usage

```
mymaximin(pool, n = 50, m = 3, iter = 1e+05, Xorig = NULL)
```

Arguments

pool, partition the base design points provided to the function
n numeric, sample size
m numeric, 3 stands for 3 components, i.e. c1, c2, and c3
iter numeric, iterations used in the stochastic sampling
Xorig matrix, initial design points

Value

Return a matrixt of the design points for the major components

```
# The case of unconstrainted experiments
library(mixexp)
num_size = 8 # num points in the design for the major component
Xorig = as.matrix(SCD(3))
# all possible combinations sum to 1
pool_3d =partitions::compositions(1000, 3,include.zero = TRUE)/1000
res_C = mymaximin(pool=pool_3d, n=num_size, m=3, iter=1e5, Xorig=Xorig)
DesignPoints(res_C,cornerlabs = c("c3","c1"),axislabs=c("c1","c2","c3"))
# The case of constrainted experiments
library(mixexp)
num_size = 8 # num points in the design for the major component
# all possible combinations sum to 1
pool_3d =partitions::compositions(1000, 3,include.zero = TRUE)/1000
c1_min=0.2
c1_max=0.45
c2_min=0.4
c2_{max}=0.6
c3_min=0.1
tmp = Xvert(nfac=3,lc=c(c1_min,c2_min,c3_min),uc =c(c1_max,c2_max,c3_max),ndm=1,pseudo=FALSE)
Xorig=tmp[c(1:6,13),c(1:3)]
colnames(Xorig)=c("V1","V2","V3")
pool_3d = t(dplyr::filter(as.data.frame(t(as.matrix(pool_3d))),t(pool_3d)[,1] > c1_min &
                     t(pool_3d)[,1] \le c1_max &
                     t(pool_3d)[,2] > c2_min &
                     t(pool_3d)[,2] \le c2_max &
                     t(pool_3d)[,3] > c3_min &
                     t(pool_3d)[,3] \le c3_max
)
res_C = mymaximin(pool=pool_3d, n=num_size, m=3, iter=1e5, Xorig=Xorig)
```

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predict.ahm

Predict method for the fitted ahm object

Description

Predict method for the fitted ahm object

Usage

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

Arguments

object ahm object

newx Matrix of new values for x at which predictions are to be made.

... not used

Value

```
predicted value(s) at newx
```

predict.cv.ahm 13

predict.cv.ahm

Predict method for the fitted cv.ahm object

Description

Predict method for the fitted cv.ahm object

Usage

```
## S3 method for class 'cv.ahm'
predict(object, newx, metric = "mse", ...)
```

not used

Arguments

. . .

object cv.ahm object

newx Matrix of new values for x at which predictions are to be made.

metric "mse" or "aicc"

Value

Return a list

```
data("pringles_fat")
data_fat = pringles_fat
h_tmp = 1.3
x = data_fat[,c("c1","c2","c3","x11","x12","x21","x22")]
y = data_fat[,1]
powerh_path = round(seq(0.001,2,length.out =15),3)
num_major = 3; dist_minor = c(2,2,1)
res = cv.ahm (y, x, powerh_path=powerh_path, metric = "mse", num_major, dist_minor, type = "weak", alpha=0, lambda_seq=seq(0,5,0.01), nfolds=NULL, mapping_type = c("power"), rep_gcv=100)
pred = predict(res)
```

pringles_fat

```
pringles_candidates2search
```

The candidate search points in the nonlinear optimization for the optimal value in the Pringles experiment

Description

The candidate search points in the nonlinear optimization for the optimal value in the Pringles experiment

Usage

```
data(pringles_candidates2search)
```

Format

matrix

Examples

```
data(pringles_candidates2search)
print(pringles_candidates2search)
```

pringles_fat

Pringles experiment data set with the percent of Fat as the response

Description

Pringles experiment data set with the percent of Fat as the response

Usage

```
data(pringles_fat)
```

Format

data.frame

References

Kang, L., Joseph, V.R. and Brenneman, W.A. (2011). Design and modeling strategies for mixture-of-mixtures experiments. *Technometrics*, 53(2), 125–36. (tandfonline)

```
data(pringles_fat)
print(pringles_fat)
```

pringles_hardness 15

pringles_hardness

Pringles experiment data set with the Hardness as the response

Description

Pringles experiment data set with the Hardness as the response

Usage

```
data(pringles_hardness)
```

Format

data.frame

References

Kang, L., Joseph, V.R. and Brenneman, W.A. (2011). Design and modeling strategies for mixture-of-mixtures experiments. *Technometrics*, 53(2), 125–36. (tandfonline)

Examples

```
data(pringles_hardness)
print(pringles_hardness)
```

summary.ahm

Summary method for the fitted ahm object

Description

Summary method for the fitted ahm object

Usage

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

Arguments

```
object fitted ahm object
```

... not used

summary.ahm

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