

Package ‘ForLion’

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Type Package

Title 'ForLion' Algorithms to Find Optimal Experimental Designs with Mixed Factors

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Maintainer Siting Lin <slin95@uic.edu>

Description

Designing experimental plans that involve both discrete and continuous factors with general parametric statistical models using the 'ForLion' algorithm and 'EW ForLion' algorithm. The algorithms will search for locally optimal designs and EW optimal designs under the D-criterion. Reference: Huang, Y., Li, K., Mandal, A., & Yang, J., (2024) <[doi:10.1007/s11222-024-10465-x](https://doi.org/10.1007/s11222-024-10465-x)>. Lin, S., Huang, Y., & Yang, J. (2025) <[doi:10.48550/arXiv.2505.00629](https://doi.org/10.48550/arXiv.2505.00629)>.

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Author Yifei Huang [aut],
Siting Lin [aut, cre],
Jie Yang [aut]

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<code>design_initial_self</code>	<i>function to generate initial design with design points and the approximate allocation</i>
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Description

function to generate initial design with design points and the approximate allocation

Usage

```
design_initial_self(
  k.continuous,
  factor.level,
  MLM,
  xlist_fix = NULL,
  lvec,
  uvec,
  bvec,
  h.func,
  link = "continuation",
  Fi.func = Fi_MLM_func,
  delta = 1e-06,
  epsilon = 1e-12,
  maxit = 1000
)
```

Arguments

<code>k.continuous</code>	number of continuous variables
<code>factor.level</code>	lower, upper limit of continuous variables, and discrete levels of categorical variables, continuous factors come first
<code>MLM</code>	TRUE or FALSE, TRUE: generate initial design for multinomial logistic model, FALSE: generate initial design for generalized linear model
<code>xlist_fix</code>	the restricted discrete settings to be chosen, default to NULL, if NULL, will generate a discrete uniform random variables
<code>lvec</code>	lower limit of continuous variables
<code>uvec</code>	upper limit of continuous variables
<code>bvec</code>	assumed parameter values of beta
<code>h.func</code>	function, is used to transfer the design point to model matrix (e.g. add interaction term, add intercept)
<code>link</code>	link function, default "continuation", other options "baseline", "adjacent" and "cumulative"
<code>Fi.func</code>	function, is used to calculate Fisher information for a design point - default to be <code>Fi_MLM_func()</code> in the package

delta	tuning parameter, the distance threshold, $\ x_i(0) - x_j(0)\ \geq \delta$
epsilon	or determining $f.\det > 0$ numerically, $f.\det \leq \epsilon$ will be considered as $f.\det \leq 0$
maxit	maximum number of iterations

Value

X matrix of initial design point
 p0 initial random approximate allocation
 f.det the determinant of Fisher information matrix for the initial design

Examples

```
k.continuous.temp=5
link.temp = "cumulative"
n.factor.temp = c(0,0,0,0,0,2) # 1 discrete factor w/ 2 levels + 5 continuous
## Note: Always put continuous factors ahead of discrete factors,
## pay attention to the order of coefficients paring with predictors
lvec.temp = c(-25,-200,-150,-100,0,-1)
uvec.temp = c(25,200,0,0,16,1)
hfunc.temp = function(y){
  if(length(y) != 6){stop("Input should have length 6");}
  model.mat = matrix(NA, nrow=5, ncol=10, byrow=TRUE)
  model.mat[5,]=0
  model.mat[1:4,1:4] = diag(4)
  model.mat[1:4, 5] =((-1)*y[6])
  model.mat[1:4, 6:10] = matrix(((1)*y[1:5]), nrow=4, ncol=5, byrow=TRUE)
  return(model.mat)
}
bvec.temp=c(-1.77994301, -0.05287782, 1.86852211, 2.76330779, -0.94437464, 0.18504420,
-0.01638597, -0.03543202, -0.07060306, 0.10347917)

design_initial_self(k.continuous=k.continuous.temp, factor.level=n.factor.temp,
MLM=TRUE,xlist_fix=NULL, lvec=lvec.temp,uvec=uvec.temp, bvec=bvec.temp,
h.func=hfunc.temp,link=link.temp)
```

<i>discrete_rv_self</i>	<i>function to generate discrete uniform random variables for initial random design points in ForLion</i>
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Description

function to generate discrete uniform random variables for initial random design points in ForLion

Usage

```
discrete_rv_self(n, xlist)
```

Arguments

n	number of discrete random variables
xlist	list of levels for variables to be generated

Value

list of discrete uniform random variables

Examples

```
n=3 #three discrete random variables
xlist=list(c(-1,1),c(-1,1),c(-1,0,1)) #two binary and one three-levels
discrete_rv_self(n, xlist)
```

dprime_func_self	<i>function to calculate du/dx in the gradient of d(x, Xi), will be used in ForLion_MLM_func() function, details see Appendix C in Huang, Li, Mandal, Yang (2024)</i>
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Description

function to calculate du/dx in the gradient of d(x, Xi), will be used in ForLion_MLM_func() function, details see Appendix C in Huang, Li, Mandal, Yang (2024)

Usage

```
dprime_func_self(
  xi,
  bvec,
  h.func,
  h.prime,
  inv.F.mat,
  Ux,
  link = "continuation",
  k.continuous
)
```

Arguments

xi	a vector of design point
bvec	parameter of the multinomial logistic regression model
h.func	function, is used to transfer xi to model matrix (e.g. add interaction term, add intercept)
h.prime	function, is used to find dX/dx

<code>inv.F.mat</code>	inverse of F_Xi matrix, inverse of fisher information of current design w/o new point
<code>Ux</code>	<code>U_x</code> matrix in the algorithm, get from <code>Fi_MLM_func()</code> function
<code>link</code>	multinomial link function, default is "continuation", other choices "baseline", "cumulative", and "adjacent"
<code>k.continuous</code>	number of continuous factors

Value

dU/dx in the gradient of sensitivity function $d(x, \Xi)$

`EW_design_initial_GLM` *function to generate a initial EW Design for generalized linear models*

Description

function to generate a initial EW Design for generalized linear models

Usage

```
EW_design_initial_GLM(
  k.continuous,
  factor.level,
  Integral_based,
  b_matrix,
  joint_Func_b,
  Lowerbounds,
  Upperbounds,
  xlist_fix = NULL,
  lvec,
  uvec,
  h.func,
  link = "continuation",
  delta = 1e-06,
  epsilon = 1e-12,
  maxit = 1000
)
```

Arguments

<code>k.continuous</code>	number of continuous variables
<code>factor.level</code>	lower, upper limit of continuous variables, and discrete levels of categorical variables, continuous factors come first
<code>Integral_based</code>	TRUE or FALSE, if TRUE then we will find the integral-based EW D-optimality otherwise we will find the sample-based EW D-optimality

b_matrix	The matrix of the sampled parameter values of beta
joint_Func_b	The prior joint probability distribution of the parameters
Lowerbounds	The lower limit of the prior distribution for each parameter
Upperbounds	The upper limit of the prior distribution for each parameter
xlist_fix	the restricted discrete settings to be chosen, default to NULL, if NULL, will generate a discrete uniform random variables
lvec	lower limit of continuous variables
uvec	upper limit of continuous variables
h.func	function, is used to transfer the design point to model matrix (e.g. add interaction term, add intercept)
link	link function, default "continuation", other options "baseline", "adjacent" and "cumulative"
delta	tuning parameter, the distance threshold, $\ x_i(0) - x_j(0) \ \geq \delta$
epsilon	determining f.det > 0 numerically, f.det <= epsilon will be considered as f.det <= 0
maxit	maximum number of iterations

Value

X matrix of initial design point
 p0 initial random approximate allocation
 f.det the determinant of the expected Fisher information matrix for the initial design

EW_design_initial_MLM *function to generate a initial EW Design for multinomial logistic models*

Description

function to generate a initial EW Design for multinomial logistic models

Usage

```
EW_design_initial_MLM(
  k.continuous,
  factor.level,
  xlist_fix = NULL,
  lvec,
  uvec,
  bvec_matrix,
  h.func,
  link = "continuation",
  EW_Fi.func = EW_Fi_MLM_func,
```

```

    delta = 1e-06,
    epsilon = 1e-12,
    maxit = 1000
)

```

Arguments

<code>k.continuous</code>	number of continuous variables
<code>factor.level</code>	lower, upper limit of continuous variables, and discrete levels of categorical variables, continuous factors come first
<code>xlist_fix</code>	the restricted discrete settings to be chosen, default to NULL, if NULL, will generate a discrete uniform random variables
<code>lvec</code>	lower limit of continuous variables
<code>uvec</code>	upper limit of continuous variables
<code>bvec_matrix</code>	the matrix of the sampled parameter values of beta
<code>h.func</code>	function, is used to transfer the design point to model matrix (e.g. add interaction term, add intercept)
<code>link</code>	link function, default "continuation", other options "baseline", "adjacent" and "cumulative"
<code>EW_Fi.func</code>	function, is used to calculate the Expectation of Fisher information for a design point - default to be <code>EW_Fi_MLM_func()</code> in the package
<code>delta</code>	tuning parameter, the distance threshold, $\ \mathbf{x}_i(0) - \mathbf{x}_j(0) \ \geq \delta$
<code>epsilon</code>	determining $f.\det > 0$ numerically, $f.\det \leq \epsilon$ will be considered as $f.\det \leq 0$
<code>maxit</code>	maximum number of iterations

Value

`X` matrix of initial design point
`p0` initial random approximate allocation
`f.det` the determinant of the expected Fisher information matrix for the initial design.

Examples

```

k.continuous.temp=1
link.temp = "continuation"
n.factor.temp = c(0)
factor.level.temp = list(c(80,200))
hfunc.temp = function(y){
  matrix(data=c(1,y,y*y,0,0,0,0,0,1,y,0,0,0,0,0), nrow=3, ncol=5, byrow=TRUE)
}
lvec.temp = 80
uvec.temp = 200
bvec_bootstrap<-matrix(c(-0.2401, -1.9292, -2.7851, -1.614,-1.162,
                           -0.0535, -0.0274, -0.0096,-0.0291, -0.04,
                           0.0004,  0.0003,  0.0002,  0.0003,  0.1,

```

```
-9.2154, -9.7576, -9.6818, -8.5139, -8.56), nrow=4, byrow=TRUE)
EW_design_initial_MLM(k.continuous=k.continuous.temp, factor.level=n.factor.temp, xlist_fix=NULL,
lvec=lvec.temp, uvec=uvec.temp, bvec_matrix=bvec_bootstrap, h.func=hfunc.temp, link=link.temp)
```

EW_dprime_func_self *function to calculate dEu/dx in the gradient of d(x, Xi), will be used in EW_ForLion_MLM_func() function*

Description

function to calculate dEu/dx in the gradient of d(x, Xi), will be used in EW_ForLion_MLM_func() function

Usage

```
EW_dprime_func_self(
  xi,
  bvec_matrix,
  h.func,
  h.prime,
  inv.F.mat,
  EUx,
  link = "continuation",
  k.continuous
)
```

Arguments

xi	a vector of design point
bvec_matrix	the matrix of the bootstrap parameter values of beta
h.func	function, is used to transfer xi to model matrix (e.g. add interaction term, add intercept)
h.prime	function, is used to find dX/dx
inv.F.mat	inverse of F_Xi matrix, inverse of the Expectation of fisher information of current design w/o new point
EUx	EU_x matrix in the algorithm, get from EW_Fi_MLM_func() function
link	link multinomial link function, default is "continuation", other choices "baseline", "cumulative", and "adjacent"
k.continuous	number of continuous factors

Value

dEU/dx in the gradient of sensitivity function d(x, Xi)

EW_Fi_MLM_func	<i>function to generate the expected fisher information at one design point xi for multinomial logit models</i>
----------------	-----------------------------------------------------------------------------------------------------------------

Description

function to generate the expected fisher information at one design point xi for multinomial logit models

Usage

```
EW_Fi_MLM_func(X_x, bvec_matrix, link = "continuation")
```

Arguments

X_x	model matrix for a specific design point x_i, X_x=h.func(xi)
bvec_matrix	the matrix of the sampled parameter values of beta
link	multinomial logit model link function name "baseline", "cumulative", "adjacent", or"continuation", default to be "continuation"

Value

F_x The expected Fisher information matrix at x_i

EU_x E(U) matrix for calculation the expected of Fisher information matrix at x_i

Examples

```
link.temp = "continuation"
xi.temp=c(80)
hfunc.temp = function(y){
matrix(data=c(1,y,y*y,0,0,0,0,0,1,y,0,0,0,0,0), nrow=3, ncol=5, byrow=TRUE)
}
X_xtemp=hfunc.temp(xi.temp)
bvec_bootstrap<-matrix(c(-0.2401, -1.9292, -2.7851, -1.614,-1.162,
-0.0535, -0.0274, -0.0096,-0.0291, -0.04,
0.0004,  0.0003,  0.0002,  0.0003,  0.1,
-9.2154, -9.7576, -9.6818, -8.5139, -8.56),nrow=4,byrow=TRUE)
EW_Fi_MLM_func(X_x=X_xtemp, bvec_matrix=bvec_bootstrap, link=link.temp)
```

EW_ForLion_GLM_Optimal*EW ForLion for generalized linear models*

Description

EW ForLion algorithm to find EW D-optimal design for GLM models with mixed factors. Reference Section 3 of Lin, Huang, Yang (2025). Factors may include discrete factors with finite number of distinct levels and continuous factors with specified interval range (min, max), continuous factors, if any, must serve as main-effects only, allowing merging points that are close enough. Continuous factors first then discrete factors, model parameters should in the same order of factors.

Usage

```
EW_ForLion_GLM_Optimal(
  n.factor,
  factor.level,
  hfunc,
  Integral_based,
  b_matrix,
  joint_Func_b,
  Lowerbounds,
  Upperbounds,
  xlist_fix = NULL,
  link,
  reltol = 1e-05,
  rel.diff = 0,
  optim_grad = TRUE,
  maxit = 100,
  random = FALSE,
  nram = 3,
  logscale = FALSE,
  rowmax = NULL,
  Xini = NULL
)
```

Arguments

n.factor	vector of numbers of distinct levels, "0" indicates continuous factors, "0"s always come first, "2" or above indicates discrete factor, "1" is not allowed
factor.level	list of distinct levels, (min, max) for continuous factor, continuous factors first, should be the same order as n.factor
hfunc	function for obtaining model matrix $h(y)$ for given design point y , y has to follow the same order as n.factor
Integral_based	TRUE or FALSE, if TRUE then we will find the integral-based EW D-optimality otherwise we will find the sample-based EW D-optimality

b_matrix	The matrix of the sampled parameter values of beta
joint_Func_b	The prior joint probability distribution of the parameters
Lowerbounds	The lower limit of the prior distribution for each parameter
Upperbounds	The upper limit of the prior distribution for each parameter
xlist_fix	the restricted discrete settings to be chosen, default to NULL, if NULL, will generate a discrete uniform random variables
link	link function, default "logit", other links: "probit", "cloglog", "loglog", "cauchit", "log", "identity"
reltol	the relative convergence tolerance, default value 1e-5
rel.diff	points with distance less than that will be merged, default value 0
optim_grad	TRUE or FALSE, default is FALSE, whether to use the analytical gradient function or numerical gradient for searching optimal new design point
maxit	the maximum number of iterations, default value 100
random	TRUE or FALSE, if TRUE then the function will run lift-one with additional "nram" number of random approximate allocation, default to be FALSE
nram	when random == TRUE, the function will run lift-one nram number of initial proportion p00, default is 3
logscale	TRUE or FALSE, if TRUE then the EW ForLion will run lift-one with logscale, which is EW_liftoneDoptimal_log_GLM_func(); if FALSE then ForLion will run EW lift-one without logscale, which is EW_liftoneDoptimal_GLM_func()
rowmax	maximum number of points in the initial design, default NULL indicates no restriction
Xini	initial list of design points, default NULL will generate random initial design points

Value

m number of design points
 x.factor matrix with rows indicating design point
 p EW D-optimal approximate allocation
 det Optimal determinant of the expected Fisher information matrix
 x.model model matrix X
 E_w vector of E_w such that E_w=diag(p*E_w)
 convergence TRUE or FALSE
 min.diff the minimum Euclidean distance between design points
 x.close a pair of design points with minimum distance

Examples

```

hfunc.temp = function(y) {c(y,1)} # y -> h(y)=(y1,1)
n.factor.temp = c(0) # 1 continuous factors
factor.level.temp = list(c(-1,1))
link.temp="logit"
paras_lowerbound<-c(0,1)
paras_upperbound<-c(1,-1)
gjoint_b<- function(x) {
  Func_b<-1/(prod(paras_upperbound-paras_lowerbound))
  ##the prior distributions are follow uniform distribution
  return(Func_b)
}
set.seed(123)
EW_ForLion_GLM_Optimal(n.factor=n.factor.temp, factor.level=factor.level.temp,
hfunc=hfunc.temp,Integral_based=TRUE,joint_Func_b=gjoint_b, Lowerbounds=paras_lowerbound,
Upperbounds=paras_upperbound, link=link.temp, reltol=1e-6, rel.diff=0.01,
optim_grad=FALSE, maxit=500, random=FALSE, nram=3, logscale=FALSE,Xini=NULL)

```

EW_ForLion_MLM_Optimal

EW ForLion function for multinomial logit models

Description

Function for EW ForLion algorithm to find EW D-optimal design under multinomial logit models with mixed factors. Reference Section 3 of Lin, Huang, Yang (2025). Factors may include discrete factors with finite number of distinct levels and continuous factors with specified interval range (min, max), continuous factors, if any, must serve as main-effects only, allowing merging points that are close enough. Continuous factors first then discrete factors, model parameters should in the same order of factors.

Usage

```

EW_ForLion_MLM_Optimal(
  J,
  n.factor,
  factor.level,
  xlist_fix = NULL,
  hfunc,
  h.prime,
  bvec_matrix,
  link = "continuation",
  EW_Fi.func = EW_Fi_MLM_func,
  delta = 1e-05,
  epsilon = 1e-12,
  reltol = 1e-05,
  rel.diff = 0,
  maxit = 100,

```

```

    random = FALSE,
    nram = 3,
    rowmax = NULL,
    Xini = NULL,
    random.initial = FALSE,
    nram.initial = 3,
    optim_grad = FALSE
)

```

Arguments

J	number of response levels in the multinomial logit model
n.factor	vector of numbers of distinct levels, "0" indicates continuous factors, "0"s always come first, "2" or above indicates discrete factor, "1" is not allowed
factor.level	list of distinct levels, (min, max) for continuous factor, continuous factors first, should be the same order as n.factor
xlist_fix	the restricted discrete settings to be chosen, default to NULL, if NULL, will generate a discrete uniform random variables
hfunc	function for obtaining model matrix h(y) for given design point y, y has to follow the same order as n.factor
h.prime	function to obtain dX/dx
bvec_matrix	the matrix of the sampled parameter values of beta
link	link function, default "continuation", other choices "baseline", "cumulative", and "adjacent"
EW_Fi.func	function to calculate row-wise Expectation of Fisher information Fi, default is EW_Fi_MLM_func
delta	tuning parameter, the generated design points distance threshold, x_i(0) - x_j(0) >= delta, default 1e-5
epsilon	determining f.det > 0 numerically, f.det <= epsilon will be considered as f.det <= 0, default 1e-12
reltol	the relative convergence tolerance, default value 1e-5
rel.diff	points with distance less than that will be merged, default value 0
maxit	the maximum number of iterations, default value 100
random	TRUE or FALSE, if TRUE then the function will run lift-one with additional "nram" number of random approximate allocation, default to be FALSE
nram	when random == TRUE, the function will run lift-one nram number of initial proportion p00, default is 3
rowmax	maximum number of points in the initial design, default NULL indicates no restriction
Xini	initial list of design points, default NULL will generate random initial design points
random.initial	TRUE or FALSE, if TRUE then the function will run EW ForLion with additional "nram.initial" number of random initial design points, default FALSE

nram.initial when random.initial == TRUE, the function will run EW ForLion algorithm with nram.initial number of initial design points Xini, default is 3
 optim_grad TRUE or FALSE, default is FALSE, whether to use the analytical gradient function or numerical gradient for searching optimal new design point

Value

m the number of design points
 x.factor matrix of experimental factors with rows indicating design point
 p the reported EW D-optimal approximate allocation
 det the determinant of the maximum Expectation of Fisher information
 convergence TRUE or FALSE, whether converge
 min.diff the minimum Euclidean distance between design points
 x.close pair of design points with minimum distance
 itmax iteration of the algorithm

Examples

```
J=3
p=5
hfunc.temp = function(y){
  matrix(data=c(1,y,y*y,0,0,0,0,0,1,y,0,0,0,0,0), nrow=3, ncol=5, byrow=TRUE)
} #hfunc is a 3*5 matrix, transfer x design matrix to model matrix for emergence of flies example

hprime.temp = function(y){
  list(matrix_1 =matrix(data=c(0, 1, 2*y, 0, 0, 0, 0, 0, 0, 0, 1, 0, 0, 0, 0, 0),
    nrow=3, ncol=5, byrow=TRUE))
}

link.temp = "continuation"
n.factor.temp = c(0) # 1 continuous factor no discrete factor in EW ForLion
factor.level.temp = list(c(80,200)) #boundary for continuous parameter in EW Forlion
bvec_bootstrap<-matrix(c(-0.2401, -1.9292, -2.7851, -1.614,-1.162,
  -0.0535, -0.0274, -0.0096,-0.0291, -0.04,
  0.0004,  0.0003,  0.0002,  0.0003,  0.1,
  -9.2154, -9.7576, -9.6818, -8.5139, -8.56),nrow=4,byrow=TRUE)
EW_ForLion_MLM_Optimal(J=J, n.factor=n.factor.temp, factor.level=factor.level.temp,
  xlist_fix=NULL, hfunc=hfunc.temp,h.prime=h.prime.temp, bvec_matrix=bvec_bootstrap,
  rel.diff=1, link=link.temp, optim_grad=FALSE)
```

Description

EW Lift-one algorithm for D-optimal approximate design

Usage

```
EW_liftoneDoptimal_GLM_func(
  X,
  E_w,
  reltol = 1e-05,
  maxit = 100,
  random = FALSE,
  nram = 3,
  p00 = NULL
)
```

Arguments

X	Model matrix, with nrow = num of design points and ncol = num of parameters
E_w	Diagonal of E_W matrix in Fisher information matrix, can be calculated EW_Xw_maineffects_self() function in the ForLion package
reltol	reltol The relative convergence tolerance, default value 1e-5
maxit	The maximum number of iterations, default value 100
random	TRUE or FALSE, if TRUE then the function will run with additional "nram" number of initial allocation p00, default to be TRUE
nram	When random == TRUE, the function will generate nram number of initial points, default is 3
p00	Specified initial design approximate allocation; default to be NULL, this will generate a random initial design

Value

- p EW D-optimal approximate allocation
- p0 Initial approximate allocation that derived the reported EW D-optimal approximate allocation
- Maximum The maximum of the determinant of the expected Fisher information matrix of the reported EW D-optimal design
- convergence Convergence TRUE or FALSE
- itmax number of the iteration

Examples

```
hfunc.temp = function(y) {c(y,1)}; # y -> h(y)=(y1,y2,y3,1)
link.temp="logit"
paras_lowerbound<-rep(-Inf, 4)
paras_upperbound<-rep(Inf, 4)
gjoint_b<- function(x) {
  mu1 <- -0.5; sigma1 <- 1
```

```

mu2 <- 0.5; sigma2 <- 1
mu3 <- 1; sigma3 <- 1
mu0 <- 1; sigma0 <- 1
d1 <- stats::dnorm(x[1], mean = mu1, sd = sigma1)
d2 <- stats::dnorm(x[2], mean = mu2, sd = sigma2)
d3 <- stats::dnorm(x[3], mean = mu3, sd = sigma3)
d4 <- stats::dnorm(x[4], mean = mu0, sd = sigma0)
return(d1 * d2 * d3 * d4)
}
x.temp=matrix(data=c(-2,-1,-3,2,-1,-3,-2,1,-3,2,1,-3,-2,-1,3,2,-1,3,-2,1,3,2,1,3),ncol=3,byrow=TRUE)
m.temp=dim(x.temp)[1]      # number of design points
p.temp=length(paras_upperbound)    # number of predictors
Xmat.temp=matrix(0, m.temp, p.temp)
EW_wvec.temp=rep(0, m.temp)
for(i in 1:m.temp) {
htemp=EW_Xw_maineffects_self(x=x.temp[i,],Integral_based=TRUE,joint_Func_b=gjoint_b,
Lowerbounds=paras_lowerbound,Upperbounds=paras_upperbound, link=link.temp,
h.func=hfunc.temp);
Xmat.temp[i,]=htemp$X;
EW_wvec.temp[i]=htemp$E_w;
}
EW_liftoneDoptimal_GLM_func(X=Xmat.temp, E_w=EW_wvec.temp, reltol=1e-8, maxit=1000,
random=TRUE, nram=3, p00=NULL)

```

EW_liftoneDoptimal_log_GLM_func*EW Lift-one algorithm for D-optimal approximate design in log scale***Description**

EW Lift-one algorithm for D-optimal approximate design in log scale

Usage

```

EW_liftoneDoptimal_log_GLM_func(
  X,
  E_w,
  reltol = 1e-05,
  maxit = 100,
  random = FALSE,
  nram = 3,
  p00 = NULL
)

```

Arguments

- | | |
|-----|---------------------------------------------------------------------------------------------------------------------------------|
| X | Model matrix, with nrow = num of design points and ncol = num of parameters |
| E_w | Diagonal of E_W matrix in Fisher information matrix, can be calculated EW_Xw_maineffects_self() function in the ForLion package |

<code>reltol</code>	reltol The relative convergence tolerance, default value 1e-5
<code>maxit</code>	The maximum number of iterations, default value 100
<code>random</code>	TRUE or FALSE, if TRUE then the function will run with additional "nram" number of initial allocation p00, default to be TRUE
<code>nram</code>	When random == TRUE, the function will generate nram number of initial points, default is 3
<code>p00</code>	Specified initial design approximate allocation; default to be NULL, this will generate a random initial design

Value

- `p` EW D-optimal approximate allocation
- `p0` Initial approximate allocation that derived the reported EW D-optimal approximate allocation
- `Maximum` The maximum of the determinant of the Fisher information matrix of the reported EW D-optimal design
- `convergence` Convergence TRUE or FALSE
- `itmax` number of the iteration

Examples

```

hfunc.temp = function(y) {c(y,1)};    # y -> h(y)=(y1,y2,y3,1)
link.temp="logit"
paras_lowerbound<-rep(-Inf, 4)
paras_upperbound<-rep(Inf, 4)
gjoint_b<- function(x) {
  mu1 <- -0.5; sigma1 <- 1
  mu2 <- 0.5; sigma2 <- 1
  mu3 <- 1; sigma3 <- 1
  mu0 <- 1; sigma0 <- 1
  d1 <- stats::dnorm(x[1], mean = mu1, sd = sigma1)
  d2 <- stats::dnorm(x[2], mean = mu2, sd = sigma2)
  d3 <- stats::dnorm(x[3], mean = mu3, sd = sigma3)
  d4 <- stats::dnorm(x[4], mean = mu0, sd = sigma0)
  return(d1 * d2 * d3 * d4)
}
x.temp=matrix(data=c(-2,-1,-3,2,-1,-3,-2,1,-3,2,1,-3,-2,-1,3,2,-1,3,-2,1,3,2,1,3),
               ncol=3,byrow=TRUE)
m.temp=dim(x.temp)[1]      # number of design points
p.temp=length(paras_upperbound)    # number of predictors
Xmat.temp=matrix(0, m.temp, p.temp)
EW_wvec.temp=rep(0, m.temp)
for(i in 1:m.temp) {
  htemp=EW_Xw_maineffects_self(x=x.temp[i,],Integral_based=TRUE,joint_Func_b=gjoint_b,
  Lowerbounds=paras_lowerbound, Upperbounds=paras_upperbound, link=link.temp,
  h.func=hfunc.temp);
  Xmat.temp[i,]=htemp$X;
  EW_wvec.temp[i]=htemp$E_w;
}
EW_liftonedOptimal_GLM_func(X=Xmat.temp, E_w=EW_wvec.temp, reltol=1e-8, maxit=1000, random=TRUE,
                             nram=3, p00=NULL)

```

EW_liftoneDoptimal_MLM_func*function of EW liftone for multinomial logit model*

Description

function of EW liftone for multinomial logit model

Usage

```
EW_liftoneDoptimal_MLM_func(
  m,
  p,
  Xi,
  J,
  thetavec_matrix,
  link = "continuation",
  reltol = 1e-05,
  maxit = 500,
  p00 = NULL,
  random = FALSE,
  nram = 3
)
```

Arguments

m	number of design points
p	number of parameters in the multinomial logit model
Xi	model matrix
J	number of response levels in the multinomial logit model
thetavec_matrix	the matrix of the sampled parameter values of beta
link	multinomial logit model link function name "baseline", "cumulative", "adjacent", or "continuation", default to be "continuation"
reltol	relative tolerance for convergence, default to 1e-5
maxit	the number of maximum iteration, default to 500
p00	specified initial approximate allocation, default to NULL, if NULL, will generate a random initial approximate allocation
random	TRUE or FALSE, if TRUE then the function will run with additional "nram" number of initial allocation p00, default to be TRUE
nram	when random == TRUE, the function will generate nram number of initial points, default is 3

Value

p reported EW D-optimal approximate allocation
 p0 the initial approximate allocation that derived the reported EW D-optimal design
 Maximum the maximum of the determinant of the expected Fisher information matrix
 Convergence TRUE or FALSE, whether the algorithm converges
 itmax maximum iterations

Examples

```
m=7
p=5
J=3
link.temp = "continuation"
factor_x=c(80,100,120,140,160,180,200)
hfunc.temp = function(y){
  matrix(data=c(1,y,y*y,0,0,0,0,0,1,y,0,0,0,0,0,0), nrow=3, ncol=5, byrow=TRUE)
}
Xi=rep(0,J*p*m); dim(Xi)=c(J,p,m)
for(i in 1:m) {
  Xi[,,i]=hfunc.temp(factor_x[i])
}
bvec_bootstrap<-matrix(c(-0.2401, -1.9292, -2.7851, -1.614,-1.162,
  -0.0535, -0.0274, -0.0096,-0.0291, -0.04,
  0.0004,  0.0003,  0.0002,  0.0003,  0.1,
  -9.2154, -9.7576, -9.6818, -8.5139, -8.56),nrow=4,byrow=TRUE)
EW_liftonDoptimal_MLM_func(m=m, p=p, Xi=Xi, J=J, thetavec_matrix=bvec_bootstrap,
link = "continuation",reltol=1e-5, maxit=500, p00=rep(1/7,7), random=FALSE, nram=3)
```

EW_Xw_maineffects_self

function for calculating $X=h(x)$ and $E_w=E(\nu(\beta^T h(x)))$ given a design point $x=(1,x_1,\dots,x_d)^T$

Description

function for calculating $X=h(x)$ and $E_w=E(\nu(\beta^T h(x)))$ given a design point $x=(1,x_1,\dots,x_d)^T$

Usage

```
EW_Xw_maineffects_self(
  x,
  Integral_based,
  joint_Func_b,
  Lowerbounds,
  Upperbounds,
```

```

  b_matrix,
  link = "logit",
  h.func = NULL
)

```

Arguments

x	x=(x1,...,xd) – design point/experimental setting
Integral_based	TRUE or FALSE, if TRUE then we will find the integral-based EW D-optimality otherwise we will find the sample-based EW D-optimality
joint_Func_b	The prior joint probability distribution of the parameters
Lowerbounds	The lower limit of the prior distribution for each parameter
Upperbounds	The upper limit of the prior distribution for each parameter
b_matrix	The matrix of the sampled parameter values of beta
link	link = "logit" – link function, default: "logit", other links: "probit", "cloglog", "loglog", "cauchit", "log"
h.func	function h(x)=(h1(x),...,hp(x)), default (1,x1,...,xd)

Value

X=h(x)=(h1(x),...,hp(x))	– a row for design matrix
E_w	= E(nu(b^t h(x)))
link	– link function applied

Examples

```

hfunc.temp = function(y) {c(y,1)};    # y -> h(y)=(y1,y2,y3,1)
link.temp="logit"
paras_lowerbound<-rep(-Inf, 4)
paras_upperbound<-rep(Inf, 4)
gjoint_b<- function(x) {
  mu1 <- -0.5; sigma1 <- 1
  mu2 <- 0.5; sigma2 <- 1
  mu3 <- 1; sigma3 <- 1
  mu0 <- 1; sigma0 <- 1
  d1 <- stats::dnorm(x[1], mean = mu1, sd = sigma1)
  d2 <- stats::dnorm(x[2], mean = mu2, sd = sigma2)
  d3 <- stats::dnorm(x[3], mean = mu3, sd = sigma3)
  d4 <- stats::dnorm(x[4], mean = mu0, sd = sigma0)
  return(d1 * d2 * d3 * d4)
}
x.temp = c(2,1,3)
EW_Xw_maineffects_self(x=x.temp,Integral_based=TRUE,joint_Func_b=gjoint_b,
Lowerbounds=paras_lowerbound,Upperbounds=paras_upperbound, link=link.temp,
h.func=hfunc.temp)

```

Fi _i _MLM_func	<i>function to generate fisher information at one design point xi for multinomial logit models</i>
---------------------------	----------------------------------------------------------------------------------------------------

Description

function to generate fisher information at one design point xi for multinomial logit models

Usage

```
Fii_MLM_func(X_x, bvec, link = "continuation")
```

Arguments

X_x	model matrix for a specific design point x_i, X_x=h.func(xi)
bvec	beta coefficients in the model
link	multinomial logit model link function name "baseline", "cumulative", "adjacent", or "continuation", default to be "continuation"

Value

F_x Fisher information matrix at x_i

U_x U matrix for calculation of Fisher information matrix at x_i (see Corollary 3.1 in Bu, Majumdar, Yang(2020))

Examples

```
# Reference minimizing surface example in supplementary material
# Section S.3 in Huang, Li, Mandal, Yang (2024)
xi.temp = c(-1, -25, 199.96, -150, -100, 16)
hfunc.temp = function(y){
  if(length(y) != 6){stop("Input should have length 6");}
  model.mat = matrix(NA, nrow=5, ncol=10, byrow=TRUE)
  model.mat[5,]=0
  model.mat[1:4,1:4] = diag(4)
  model.mat[1:4, 5] =((-1)*y[6])
  model.mat[1:4, 6:10] = matrix((((-1)*y[1:5])), nrow=4, ncol=5, byrow=TRUE)
  return(model.mat)
}
X_x.temp = hfunc.temp(xi.temp)
bvec.temp = c(-1.77994301, -0.05287782, 1.86852211, 2.76330779, -0.94437464,
0.18504420, -0.01638597, -0.03543202, -0.07060306, 0.10347917)
link.temp = "cumulative"
Fii_MLM_func(X_x=X_x.temp, bvec=bvec.temp, link=link.temp)
```

Description

ForLion algorithm to find D-optimal design for GLM models with mixed factors, reference: Section 4 in Huang, Li, Mandal, Yang (2024). Factors may include discrete factors with finite number of distinct levels and continuous factors with specified interval range (min, max), continuous factors, if any, must serve as main-effects only, allowing merging points that are close enough. Continuous factors first then discrete factors, model parameters should in the same order of factors.

Usage

```
ForLion_GLM_Optimal(
  n.factor,
  factor.level,
  xlist_fix = NULL,
  hfunc,
  bvec,
  link,
  reltol = 1e-05,
  rel.diff = 0,
  maxit = 100,
  random = FALSE,
  nram = 3,
  logscale = FALSE,
  rowmax = NULL,
  Xini = NULL
)
```

Arguments

<code>n.factor</code>	vector of numbers of distinct levels, "0" indicates continuous factors, "0"s always come first, "2" or above indicates discrete factor, "1" is not allowed
<code>factor.level</code>	list of distinct levels, (min, max) for continuous factor, continuous factors first, should be the same order as <code>n.factor</code>
<code>xlist_fix</code>	the restricted discrete settings to be chosen, default to <code>NULL</code> , if <code>NULL</code> , will generate a discrete uniform random variables
<code>hfunc</code>	function for obtaining model matrix $h(y)$ for given design point y , y has to follow the same order as <code>n.factor</code>
<code>bvec</code>	assumed parameter values of model parameters beta, same length of $h(y)$
<code>link</code>	link function, default "logit", other links: "probit", "cloglog", "loglog", "cauchit", "log", "identity"
<code>reltol</code>	the relative convergence tolerance, default value <code>1e-5</code>
<code>rel.diff</code>	points with distance less than that will be merged, default value 0

maxit	the maximum number of iterations, default value 100
random	TRUE or FALSE, if TRUE then the function will run lift-one with additional "nram" number of random approximate allocation, default to be FALSE
nram	when random == TRUE, the function will run lift-one nram number of initial proportion p00, default is 3
logscale	TRUE or FALSE, if TRUE then the ForLion will run lift-one with logscale, which is liftoneDoptimal_log_GLM_func(); if FALSE then ForLion will run lift-one without logscale, which is liftoneDoptimal_GLM_func()
rowmax	maximum number of points in the initial design, default NULL indicates no restriction
Xini	initial list of design points, default NULL will generate random initial design points

Value

m number of design points
x.factor matrix with rows indicating design point
p D-optimal approximate allocation
det Optimal determinant of Fisher information matrix
convergence TRUE or FALSE
min.diff the minimum Euclidean distance between design points
x.close a pair of design points with minimum distance
itmax iteration of the algorithm

Examples

```
#Example 3 in Huang, Li, Mandal, Yang (2024), electrostatic discharge experiment
hfunc.temp = function(y) {c(y,y[4]*y[5],1)}; # y -> h(y)=(y1,y2,y3,y4,y5,y4*y5,1)
n.factor.temp = c(0, 2, 2, 2, 2) # 1 continuous factor with 4 discrete factors
factor.level.temp = list(c(25,45),c(-1,1),c(-1,1),c(-1,1),c(-1,1))
link.temp="logit"
b.temp = c(0.3197169, 1.9740922, -0.1191797, -0.2518067, 0.1970956, 0.3981632, -7.6648090)
ForLion_GLM_Optimal(n.factor=n.factor.temp, factor.level=factor.level.temp, xlist_fix=NULL,
hfunc=hfunc.temp, bvec=b.temp, link=link.temp, reltol=1e-2, rel.diff=0.03, maxit=500,
random=FALSE,nram=3, logscale=TRUE)
```

Description

Function for ForLion algorithm to find D-optimal design under multinomial logit models with mixed factors. Reference Section 3 of Huang, Li, Mandal, Yang (2024). Factors may include discrete factors with finite number of distinct levels and continuous factors with specified interval range (min, max), continuous factors, if any, must serve as main-effects only, allowing merging points that are close enough. Continuous factors first then discrete factors, model parameters should in the same order of factors.

Usage

```
ForLion_MLM_Optimal(
  J,
  n.factor,
  factor.level,
  xlist_fix = NULL,
  hfunc,
  h.prime,
  bvec,
  link = "continuation",
  Fi.func = Fi_MLM_func,
  delta = 1e-05,
  epsilon = 1e-12,
  reltol = 1e-05,
  rel.diff = 0,
  maxit = 100,
  random = FALSE,
  nram = 3,
  rowmax = NULL,
  Xini = NULL,
  random.initial = FALSE,
  nram.initial = 3,
  optim.grad = FALSE
)
```

Arguments

J	number of response levels in the multinomial logit model
n.factor	vector of numbers of distinct levels, "0" indicates continuous factors, "0"s always come first, "2" or above indicates discrete factor, "1" is not allowed
factor.level	list of distinct levels, (min, max) for continuous factor, continuous factors first, should be the same order as n.factor
xlist_fix	the restricted discrete settings to be chosen, default to NULL, if NULL, will generate a discrete uniform random variables
hfunc	function for obtaining model matrix h(y) for given design point y, y has to follow the same order as n.factor
h.prime	function to obtain dX/dx
bvec	assumed parameter values of model parameters beta, same length of h(y)

link	link function, default "continuation", other choices "baseline", "cumulative", and "adjacent"
Fi.func	function to calculate row-wise Fisher information Fi, default is Fi_MLM_func
delta	tuning parameter, the generated design pints distance threshold, $\ x_i(0) - x_j(0)\ \geq delta$, default 1e-5
epsilon	for determining $f.det > 0$ numerically, $f.det \leq epsilon$ will be considered as $f.det \leq 0$, default 1e-12
reltol	the relative convergence tolerance, default value 1e-5
rel.diff	points with distance less than that will be merged, default value 0
maxit	the maximum number of iterations, default value 100
random	TRUE or FALSE, if TRUE then the function will run lift-one with additional "nram" number of random approximate allocation, default to be FALSE
nram	when random == TRUE, the function will run lift-one nram number of initial proportion p00, default is 3
rowmax	maximum number of points in the initial design, default NULL indicates no restriction
Xini	initial list of design points, default NULL will generate random initial design points
random.initial	TRUE or FALSE, if TRUE then the function will run ForLion with additional "nram.initial" number of random initial design points, default FALSE
nram.initial	when random.initial == TRUE, the function will run ForLion algorithm with nram.initial number of initial design points Xini, default is 3
optim_grad	TRUE or FALSE, default is FALSE, whether to use the analytical gradient function or numerical gradient for searching optimal new design point

Value

- m the number of design points
- x.factor matrix of experimental factors with rows indicating design point
- p the reported D-optimal approximate allocation
- det the determinant of the maximum Fisher information
- convergence TRUE or FALSE, whether converge
- min.diff the minimum Euclidean distance between design points
- x.close pair of design points with minimum distance
- itmax iteration of the algorithm

Examples

```

m=5
p=10
J=5
link.temp = "cumulative"
n.factor.temp = c(0,0,0,0,0,2) # 1 discrete factor w/ 2 levels + 5 continuous

```

```

## Note: Always put continuous factors ahead of discrete factors,
## pay attention to the order of coefficients paring with predictors
factor.level.temp = list(c(-25,25), c(-200,200),c(-150,0),c(-100,0),c(0,16),c(-1,1))
hfunc.temp = function(y){
  if(length(y) != 6){stop("Input should have length 6");}
  model.mat = matrix(NA, nrow=5, ncol=10, byrow=TRUE)
  model.mat[5,]=0
  model.mat[1:4,1:4] = diag(4)
  model.mat[1:4, 5] =((-1)*y[6])
  model.mat[1:4, 6:10] = matrix(((1)*y[1:5]), nrow=4, ncol=5, byrow=TRUE)
  return(model.mat)
}
bvec.temp=c(-1.77994301, -0.05287782, 1.86852211, 2.76330779, -0.94437464, 0.18504420,
-0.01638597, -0.03543202, -0.07060306, 0.10347917)

h.prime.temp = NULL #use numerical gradient (optim_grad=FALSE)
ForLion_MLM_Optimal(J=J, n.factor=n.factor.temp, factor.level=factor.level.temp, xlist_fix=NULL,
hfunc=hfunc.temp,h.prime=h.prime.temp, bvec=bvec.temp, link=link.temp, optim_grad=FALSE)

```

GLM_Exact_Design*rounding algorithm for generalized linear models***Description**

rounding algorithm for generalized linear models

Usage

```
GLM_Exact_Design(
  k.continuous,
  design_x,
  design_p,
  det.design,
  p,
  ForLion,
  bvec,
  Integral_based,
  b_matrix,
  joint_Func_b,
  Lowerbounds,
  Upperbounds,
  rel.diff,
  L,
  N,
  hfunc,
  link
)
```

Arguments

<code>k.continuous</code>	number of continuous factors
<code>design_x</code>	the matrix with rows indicating design point which we got from the approximate design
<code>design_p</code>	the corresponding approximate allocation
<code>det.design</code>	the determinant of the approximate design
<code>p</code>	number of parameters
<code>ForLion</code>	TRUE or FALSE, TRUE: this approximate design was generated by ForLion algorithm, FALSE: this approximate was generated by EW ForLion algorithm
<code>bvec</code>	If ForLion==TRUE assumed parameter values of model parameters beta, same length of <code>h(y)</code>
<code>Integral_based</code>	TRUE or FALSE, if TRUE then we will find the integral-based EW D-optimality otherwise we will find the sample-based EW D-optimality
<code>b_matrix</code>	The matrix of the sampled parameter values of beta
<code>joint_Func_b</code>	The prior joint probability distribution of the parameters
<code>Lowerbounds</code>	The lower limit of the prior distribution for each parameter
<code>Upperbounds</code>	The upper limit of the prior distribution for each parameter
<code>rel.diff</code>	points with distance less than that will be merged
<code>L</code>	vector: rounding factors
<code>N</code>	total number of observations
<code>hfunc</code>	function for obtaining model matrix <code>h(y)</code> for given design point <code>y</code> , <code>y</code> has to follow the same order as <code>n.factor</code>
<code>link</code>	link function, default "logit", other links: "probit", "cloglog", "loglog", "cauchit", "log", "identity"

Value

`x.design` matrix with rows indicating design point
`ni.design` exact allocation
`rel.efficiency` relative efficiency of the Exact and Approximate Designs

Examples

```

k.continuous=1
design_x=matrix(c(25, -1, -1,-1, -1 ,
                  25, -1, -1, -1, 1,
                  25, -1, -1, 1, -1,
                  25, -1, -1, 1, 1,
                  25, -1, 1, -1, -1,
                  25, -1, 1, -1, 1,
                  25, -1, 1, 1, -1,
                  25, -1, 1, 1, 1,
                  25, 1, -1, 1, -1,
                  25, 1, 1, -1, -1,
```

```

25, 1, 1, -1, 1,
25, 1, 1, 1, -1,
25, 1, 1, 1, 1,
38.9479, -1, 1, 1, -1,
34.0229, -1, 1, -1, -1,
35.4049, -1, 1, -1, 1,
37.1960, -1, -1, 1, -1,
33.0884, -1, 1, 1, 1),nrow=18,ncol=5,byrow = TRUE)
hfunc.temp = function(y) {c(y,y[4]*y[5],1)};    # y -> h(y)=(y1,y2,y3,y4,y5,y4*y5,1)
link.temp="logit"
design_p=c(0.0848, 0.0875, 0.0410, 0.0856, 0.0690, 0.0515,
          0.0901, 0.0845, 0.0743, 0.0356, 0.0621, 0.0443,
          0.0090, 0.0794, 0.0157, 0.0380, 0.0455, 0.0022)
det.design=4.552715e-06
paras_lowerbound<-c(0.25,1,-0.3,-0.3,0.1,0.35,-8.0)
paras_upperbound<-c(0.45,2,-0.1,0.0,0.4,0.45,-7.0)
gjoint_b<- function(x) {
  Func_b<-1/(prod(paras_upperbound-paras_lowerbound))
  ##the prior distributions are follow uniform distribution
  return(Func_b)
}
GLM_Exact_Design(k.continuous=k.continuous,design_x=design_x,
design_p=design_p,det.design=det.design,p=7,ForLion=FALSE,Integral_based=TRUE,
joint_Func_b=gjoint_b,Lowerbounds=paras_lowerbound, Upperbounds=paras_upperbound,
rel.diff=0,L=1,N=100,hfunc=hfunc.temp,link=link.temp)

```

liftoneDoptimal_GLM_func*Lift-one algorithm for D-optimal approximate design***Description**

Lift-one algorithm for D-optimal approximate design

Usage

```
liftoneDoptimal_GLM_func(
  X,
  w,
  reltol = 1e-05,
  maxit = 100,
  random = FALSE,
  nram = 3,
  p00 = NULL
)
```

Arguments

X	Model matrix, with nrow = num of design points and ncol = num of parameters
---	-----------------------------------------------------------------------------

w	Diagonal of W matrix in Fisher information matrix, can be calculated Xw_maineffects_self() function in the ForLion package
reltol	The relative convergence tolerance, default value 1e-5
maxit	The maximum number of iterations, default value 100
random	TRUE or FALSE, if TRUE then the function will run with additional "nram" number of initial allocation p00, default to be TRUE
nram	When random == TRUE, the function will generate nram number of initial points, default is 3
p00	Specified initial design approximate allocation; default to be NULL, this will generate a random initial design

Value

- p D-optimal approximate allocation
 p0 Initial approximate allocation that derived the reported D-optimal approximate allocation
 Maximum The maximum of the determinant of the Fisher information matrix of the reported D-optimal design
 convergence Convergence TRUE or FALSE
 itmax number of the iteration

Examples

```

hfunc.temp = function(y) {c(y,y[4]*y[5],1)};    # y -> h(y)=(y1,y2,y3,y4,y5,y4*y5,1)
link.temp="logit"
x.temp = matrix(data=c(25.00000,1,-1,1,-1,25.00000,1,1,1,-1,32.06741,-1,1,-1,1,40.85698,
-1,1,1,-1,28.86602,-1,1,-1,-1,29.21486,-1,-1,1,1,25.00000,1,1,1,1, 25.00000,1,1,-1,-1),
ncol=5, byrow=TRUE)
b.temp = c(0.3197169, 1.9740922, -0.1191797, -0.2518067, 0.1970956, 0.3981632, -7.6648090)
X.mat = matrix(,nrow=8, ncol=7)
w.vec = rep(NA,8)
for(i in 1:8) {
  htemp=Xw_maineffects_self(x=x.temp[i,], b=b.temp, link=link.temp, h.func=hfunc.temp);
  X.mat[i,]=htemp$X;
  w.vec[i]=htemp$w;
}
liftoneDoptimal_GLM_func(X=X.mat, w=w.vec, reltol=1e-5, maxit=500, random=TRUE, nram=3, p00=NULL)

```

liftoneDoptimal_log_GLM_func

Lift-one algorithm for D-optimal approximate design in log scale

Description

Lift-one algorithm for D-optimal approximate design in log scale

Usage

```
liftoneDoptimal_log_GLM_func(
  X,
  w,
  reltol = 1e-05,
  maxit = 100,
  random = FALSE,
  nram = 3,
  p00 = NULL
)
```

Arguments

X	Model matrix, with nrow = num of design points and ncol = num of parameters
w	Diagonal of W matrix in Fisher information matrix, can be calculated Xw_maineffects_self() function in the ForLion package
reltol	The relative convergence tolerance, default value 1e-5
maxit	The maximum number of iterations, default value 100
random	TRUE or FALSE, if TRUE then the function will run with additional "nram" number of initial allocation p00, default to be TRUE
nram	When random == TRUE, the function will generate nram number of initial points, default is 3
p00	Specified initial design approximate allocation; default to be NULL, this will generate a random initial design

Value

p	D-optimal approximate allocation
p0	Initial approximate allocation that derived the reported D-optimal approximate allocation
Maximum	The maximum of the determinant of the expected Fisher information matrix of the reported D-optimla design
convergence	Convergence TRUE or FALSE
itmax	number of the iteration

Examples

```
hfunc.temp = function(y) {c(y,y[4]*y[5],1)};    # y -> h(y)=(y1,y2,y3,y4,y5,y4*y5,1)
link.temp="logit"
x.temp = matrix(data=c(25.00000,1,-1,1,-1,25.00000,1,1,1,-1,32.06741,-1,1,-1,1,40.85698,
-1,1,1,-1,28.86602,-1,1,-1,-1,29.21486,-1,-1,1,1,25.00000,1,1,1,1, 25.00000,1,1,-1,-1),
ncol=5, byrow=TRUE)
b.temp = c(0.3197169, 1.9740922, -0.1191797, -0.2518067, 0.1970956, 0.3981632, -7.6648090)
X.mat = matrix(,nrow=8, ncol=7)
w.vec = rep(NA,8)
for(i in 1:8) {
  htemp=Xw_maineffects_self(x=x.temp[i,], b=b.temp, link=link.temp, h.func=hfunc.temp);
```

```
X.mat[i,]=htemp$X;
w.vec[i]=htemp$w;
};
liftoneDoptimal_log_GLM_func(X=X.mat, w=w.vec, reltol=1e-5, maxit=500,
random=TRUE, nram=3, p00=NULL)
```

liftoneDoptimal_MLM_func*function of liftone for multinomial logit model***Description**

function of liftone for multinomial logit model

Usage

```
liftoneDoptimal_MLM_func(
  m,
  p,
  Xi,
  J,
  thetavec,
  link = "continuation",
  reltol = 1e-05,
  maxit = 500,
  p00 = NULL,
  random = FALSE,
  nram = 3
)
```

Arguments

m	number of design points
p	number of parameters in the multinomial logit model
Xi	model matrix
J	number of response levels in the multinomial logit model
thetavec	model parameter
link	multinomial logit model link function name "baseline", "cumulative", "adjacent", or "continuation", default to be "continuation"
reltol	relative tolerance for convergence, default to 1e-5
maxit	the number of maximum iteration, default to 500
p00	specified initial approximate allocation, default to NULL, if NULL, will generate a random initial approximate allocation
random	TRUE or FALSE, if TRUE then the function will run with additional "nram" number of initial allocation p00, default to be TRUE
nram	when random == TRUE, the function will generate nram number of initial points, default is 3

Value

p reported D-optimal approximate allocation
 p0 the initial approximate allocation that derived the reported D-optimal design
 Maximum the maximum of the determinant of the Fisher information matrix
 Convergence TRUE or FALSE, whether the algorithm converges
 itmax maximum iterations

Examples

```

m=5
p=10
J=5
factor_x = matrix(c(-1,-25,199.96,-150,-100,16,1,23.14,196.35,0,-100,
16,1,-24.99,199.99,-150,0,16,-1,25,-200,0,0,16,-1,-25,-200,-150,0,16),ncol=6,byrow=TRUE)
Xi=rep(0,J*p*m); dim(Xi)=c(J,p,m)
hfunc.temp = function(y){
  if(length(y) != 6){stop("Input should have length 6");}
  model.mat = matrix(NA, nrow=5, ncol=10, byrow=TRUE)
  model.mat[5,]=0
  model.mat[1:4,1:4] = diag(4)
  model.mat[1:4, 5] =((-1)*y[6])
  model.mat[1:4, 6:10] = matrix((((-1)*y[1:5])), nrow=4, ncol=5, byrow=TRUE)
  return(model.mat)
}
for(i in 1:m) {
  Xi[,i]=hfunc.temp(factor_x[i,])
}
thetavec=c(-1.77994301, -0.05287782,  1.86852211, 2.76330779, -0.94437464, 0.18504420,
-0.01638597, -0.03543202, -0.07060306, 0.10347917)
liftoneOptimal MLM_func(m=m,p=p,Xi=Xi,J=J,thetavec=thetavec,
link="cumulative",p00=rep(1/5,5), random=FALSE)

```

MLM_Exact_Design *rounding algorithm for multinomial logit models*

Description

rounding algorithm for multinomial logit models

Usage

```
MLM_Exact_Design(
  J,
  k.continuous,
  design_x,
  design_p,
  det.design,
```

```

p,
ForLion,
bvec,
bvec_matrix,
rel.diff,
L,
N,
hfunc,
link
)

```

Arguments

J	number of response levels in the multinomial logit model
k.continuous	number of continuous factors
design_x	the matrix with rows indicating design point which we got from the approximate design
design_p	the corresponding approximate allocation
det.design	the determinant of the approximate design
p	number of parameters
ForLion	TRUE or FALSE, TRUE: this approximate design was generated by ForLion algorithm, FALSE: this approximate was generated by EW ForLion algorithm
bvec	If ForLion==TRUE assumed parameter values of model parameters beta, same length of h(y)
bvec_matrix	If ForLion==FALSE the matrix of the sampled parameter values of beta
rel.diff	points with distance less than that will be merged
L	vector: rounding factors
N	total number of observations
hfunc	function for obtaining model matrix h(y) for given design point y, y has to follow the same order as n.factor
link	link function, default "continuation", other choices "baseline", "cumulative", and "adjacent"

Value

- x.design matrix with rows indicating design point
- ni.design exact allocation
- rel.efficiency relative efficiency of the Exact and Approximate Designs

Examples

```

J=3
k.continuous=1
design_x<-c(0.0000,103.5451,149.2355)
design_p<-c(0.2027, 0.3981, 0.3992)

```

```

det.design=54016609
p=5
theta = c(-1.935, -0.02642, 0.0003174, -9.159, 0.06386)
hfunc.temp = function(y){
  matrix(data=c(1,y,y*y,0,0,0,0,0,1,y,0,0,0,0,0), nrow=3,
         ncol=5, byrow=TRUE)
}
link.temp = "continuation"
MLM_Exact_Design(J=J, k.continuous=k.continuous,design_x=design_x,
design_p=design_p,det.design=det.design,p=p,ForLion=TRUE,bvec=theta,
rel.diff=1,L=0.5,N=1000,hfunc=hfunc.temp,link=link.temp)

```

nu1_cauchit_self *function to calculate first derivative of nu function given eta for cauchit link*

Description

function to calculate first derivative of nu function given eta for cauchit link

Usage

```
nu1_cauchit_self(x)
```

Arguments

x	vector of eta, eta=X*beta
---	---------------------------

Value

the first derivative of nu function given eta for cauchit link

Examples

```

eta = c(1,2,3,4)
nu1_cauchit_self(eta)

```

nu1_identity_self *function to calculate first derivative of nu function given eta for identity link*

Description

function to calculate first derivative of nu function given eta for identity link

Usage

```
nu1_identity_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the first derivative of nu function given eta for identity link

Examples

```
eta = c(1,2,3,4)
nu1_identity_self(eta)
```

nu1_logit_self *function to calculate the first derivative of nu function given eta for logit link*

Description

function to calculate the first derivative of nu function given eta for logit link

Usage

```
nu1_logit_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the first derivative of nu function given eta for logit link

Examples

```
eta = c(1,2,3,4)
nu1_logit_self(eta)
```

nu1_loglog_self *function to calculate the first derivative of nu function given eta for log-log link*

Description

function to calculate the first derivative of nu function given eta for log-log link

Usage

```
nu1_loglog_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the first derivative of nu function given eta for log-log link

Examples

```
eta = c(1,2,3,4)
nu1_loglog_self(eta)
```

nu1_log_self *function to calculate first derivative of nu function given eta for log link*

Description

function to calculate first derivative of nu function given eta for log link

Usage

```
nu1_log_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the first derivative of nu function given eta for log link

Examples

```
eta = c(1,2,3,4)
nu1_log_self(eta)
```

nu1_probit_self

function to calculate the first derivative of nu function given eta for probit link

Description

function to calculate the first derivative of nu function given eta for probit link

Usage

```
nu1_probit_self(x)
```

Arguments

x	vector of eta, eta=X*beta
---	---------------------------

Value

the first derivative of nu function for probit link

Examples

```
eta = c(1,2,3,4)
nu1_probit_self(eta)
```

nu2_cauchit_self

function to calculate the second derivative of nu function given eta for cauchit link

Description

function to calculate the second derivative of nu function given eta for cauchit link

Usage

```
nu2_cauchit_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the second derivative of nu function for cauchit link

Examples

```
eta = c(1,2,3,4)
nu2_cauchit_self(eta)
```

nu2_identity_self *function to calculate the second derivative of nu function given eta for identity link*

Description

function to calculate the second derivative of nu function given eta for identity link

Usage

```
nu2_identity_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the second derivative of nu function for identity link

Examples

```
eta = c(1,2,3,4)
nu2_identity_self(eta)
```

nu2_logit_self *function to calculate the second derivative of nu function given eta for logit link*

Description

function to calculate the second derivative of nu function given eta for logit link

Usage

```
nu2_logit_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the second derivative of nu function for logit link

Examples

```
eta = c(1,2,3,4)
nu2_logit_self(eta)
```

nu2_loglog_self *function to calculate the second derivative of nu function given eta for loglog link*

Description

function to calculate the second derivative of nu function given eta for loglog link

Usage

```
nu2_loglog_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the second derivative of nu function for loglog link

Examples

```
eta = c(1,2,3,4)
nu2_loglog_self(eta)
```

nu2_log_self

function to calculate the second derivative of nu function given eta for log link

Description

function to calculate the second derivative of nu function given eta for log link

Usage

```
nu2_log_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the second derivative of nu function for log link

Examples

```
eta = c(1,2,3,4)
nu2_log_self(eta)
```

nu2_probit_self

function to calculate the second derivative of nu function given eta for probit link

Description

function to calculate the second derivative of nu function given eta for probit link

Usage

```
nu2_probit_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

the second derivative of nu function for probit link

Examples

```
eta = c(1,2,3,4)
nu2_probit_self(eta)
```

nu_cauchit_self

function to calculate w = nu(eta) given eta for cauchit link

Description

function to calculate $w = \text{nu}(\text{eta})$ given eta for cauchit link

Usage

```
nu_cauchit_self(x)
```

Arguments

x a list of eta = X*beta

Value

diagonal element of W matrix which is nu(eta)

Examples

```
eta = c(1,2,3,4)
nu_cauchit_self(eta)
```

nu_identity_self

function to calculate w = nu(eta) given eta for identity link

Description

function to calculate $w = \text{nu}(\text{eta})$ given eta for identity link

Usage

```
nu_identity_self(x)
```

Arguments

x Numeric vector of eta, eta = X*beta.

Value

A numeric vector representing the diagonal elements of the W matrix (nu(eta)).

Examples

```
eta = c(1,2,3,4)
nu_identity_self(eta)
```

nu_logit_self *function to calculate w = nu(eta) given eta for logit link*

Description

function to calculate w = nu(eta) given eta for logit link

Usage

```
nu_logit_self(x)
```

Arguments

x vector of eta, eta=X*beta

Value

diagonal element of W matrix which is nu(eta)

Examples

```
eta = c(1,2,3,4)
nu_logit_self(eta)
```

nu_loglog_self*function to calculate w = nu(eta) given eta for loglog link***Description**

function to calculate $w = \text{nu}(\eta)$ given η for loglog link

Usage

```
nu_loglog_self(x)
```

Arguments

x vector of η , $\eta = X^* \beta$

Value

diagonal element of W matrix which is $\text{nu}(\eta)$

Examples

```
eta = c(1,2,3,4)
nu_loglog_self(eta)
```

nu_log_self*function to calculate w = nu(eta) given eta for log link***Description**

function to calculate $w = \text{nu}(\eta)$ given η for log link

Usage

```
nu_log_self(x)
```

Arguments

x Numeric vector of η , $\eta = X^* \beta$.

Value

A numeric vector representing the diagonal elements of the W matrix ($\text{nu}(\eta)$).

Examples

```
eta = c(1,2,3,4)
nu_log_self(eta)
```

nu_probit_self

*function to calculate w = nu(eta) given eta for probit link***Description**

function to calculate w = nu(eta) given eta for probit link

Usage

```
nu_probit_self(x)
```

Arguments

x	vector of eta, eta=X*beta
---	---------------------------

Value

diagonal element of W matrix which is nu(eta)

Examples

```
eta = c(1,2,3,4)
nu_probit_self(eta)
```

polynomial_sol_J3

*functions to solve 2th order polynomial function given coefficients***Description**

functions to solve 2th order polynomial function given coefficients

Usage

```
polynomial_sol_J3(c0, c1, c2)
```

Arguments

c0	constant coefficient of polynomial function
c1	coefficient of 1st order term
c2	coefficient of 2nd order term

Value

sol the 2 solutions of the polynomial function

Examples

```
polynomial_sol_J3(-2,-3, 1)
```

```
polynomial_sol_J4
```

functions to solve 3th order polynomial function given coefficients

Description

functions to solve 3th order polynomial function given coefficients

Usage

```
polynomial_sol_J4(c0, c1, c2, c3)
```

Arguments

c0	constant coefficient of polynomial function
c1	coefficient of 1st order term
c2	coefficient of 2nd order term
c3	coefficient of 3rd order term

Value

sol the 3 solutions of the polynomial function

Examples

```
polynomial_sol_J4(0,9,6,1)
```

`polynomial_sol_J5` *functions to solve 4th order polynomial function given coefficients*

Description

functions to solve 4th order polynomial function given coefficients

Usage

```
polynomial_sol_J5(c0, c1, c2, c3, c4)
```

Arguments

<code>c0</code>	constant coefficient of polynomial function
<code>c1</code>	coefficient of 1st order term
<code>c2</code>	coefficient of 2nd order term
<code>c3</code>	coefficient of 3rd order term
<code>c4</code>	coefficient of 4th order term

Value

`sol` the 4 solutions of the polynomial function

Examples

```
polynomial_sol_J5(19, -53, 19, -21, 30)
```

`print.design_output` *Print Method for Design Output from ForLion Algorithms*

Description

Custom print method for a list containing design information.

Usage

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

Arguments

<code>x</code>	An object of class ‘ <code>design_output</code> ’.
<code>...</code>	Additional arguments (ignored).

Value

Invisibly returns ‘`x`’.

<code>print.list_output</code>	<i>Print Method for list_output Objects</i>
--------------------------------	---------------------------------------------

Description

Custom print method for objects of class ‘list_output‘.

Usage

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

Arguments

<code>x</code>	An object of class ‘list_output‘.
<code>...</code>	Additional arguments (ignored).

Value

Invisibly returns ‘x‘ (the input object).

<code>svd_inverse</code>	<i>SVD Inverse Of A Square Matrix</i>
--------------------------	---------------------------------------

Description

This function returns the inverse of a matrix using singular value decomposition. If the matrix is a square matrix, this should be equivalent to using the solve function. If the matrix is not a square matrix, then the result is the Moore-Penrose pseudo inverse.

Usage

```
svd_inverse(x)
```

Arguments

<code>x</code>	the matrix for calculation of inverse
----------------	---------------------------------------

Value

the inverse of the matrix x

Examples

```
x = diag(4)
svd_inverse(x)
```

xmat_discrete_self *Generate initial designs within ForLion algorithms*

Description

Generate initial designs within ForLion algorithms

Usage

```
xmat_discrete_self(xlist, rowmax = NULL)
```

Arguments

- | | |
|--------|------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| xlist | a list of factor levels within ForLion algorithms, for example, a binary factor might be c(-1,1), a continuous factor within range of (25,45) will be c(25, 45). |
| rowmax | maximum number of rows of the design matrix |

Value

design matrix of all possible combinations of discrete factors levels with min and max of the continuous factors.

Examples

```
#define list of factor levels for one continuous factor, four binary factors
factor.level.temp = list(c(25,45),c(-1,1),c(-1,1),c(-1,1),c(-1,1))
xmat_discrete_self(xlist = factor.level.temp)
```

Xw_maineffects_self *function for calculating X=h(x) and w=nu(beta^T h(x)) given a design point x = (x1,...,xd)^T*

Description

function for calculating X=h(x) and w=nu(beta^T h(x)) given a design point x = (x1,...,xd)^T

Usage

```
Xw_maineffects_self(x, b, link = "logit", h.func = NULL)
```

Arguments

x	x=(x1,...,xd) – design point/experimental setting
b	b=(b1,...,bp) – assumed parameter values
link	link = "logit" – link function, default: "logit", other links: "probit", "cloglog", "loglog", "cauchit", "log", and "identity"
h.func	function h(x)=(h1(x),...,hp(x)), default (1,x1,...,xd)

Value

X=h(x)=(h1(x),...,hp(x)) – a row for design matrix
 w – nu(b^t h(x))
 link – link function applied

Examples

```
# y -> h(y)=(y1,y2,y3,y4,y5,y4*y5,1) in hfunc
hfunc.temp = function(y) {c(y,y[4]*y[5],1)};
link.temp="logit"
x.temp = c(25,1,1,1,1)
b.temp = c(-7.533386, 1.746778, -0.1937022, -0.09704664, 0.1077859, 0.2729715, 0.4293171)
Xw_maineffects_self(x.temp, b.temp, link=link.temp, h.func=hfunc.temp)
```

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