# Package 'ForLion'

## February 11, 2025

design\_initial\_self

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## Description

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

approximate allocation

design\_initial\_self 3

## Usage

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

## Arguments

k.continuous	number of continuous variables
factor.level	lower, upper limit of continuous variables, and discrete levels of categorical variables, continuous factors come first
lvec	lower limit of continuous variables
uvec	upper limit of continuous variables
bvec	assumed parameter values of beta
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"
Fi.func	function, is used to calculate Fisher inforantion for a design point - default to be $Fi\_MLM\_func()$ in the package
delta	tuning parameter, the distance threshold, $\  \mathbf{x}_{i}(0) - \mathbf{x}_{j}(0) \  \ge delta$
epsilon	or 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 Fisher information matrix for the random initial design

```
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
```

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```
## 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)
{\tt design\_initial\_self(k.continuous=k.continuous.temp,\ factor.level=n.factor.temp,\ lvec=lvec.temp,\ lvec
uvec=uvec.temp, bvec=bvec.temp, h.func=hfunc.temp, link=link.temp)
```

discrete\_rv\_self

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

#### **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 variablesxlist list of levels for variables to be generated

#### Value

list of discrete uniform random variables

```
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 5

dprime_func_self	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)
	Manadi, Tang (2024)

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

#### Value

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

```
{\sf EW\_design\_initial\_self}
```

function to generate random initial design with design points and the approximate allocation (For EW)

## Description

function to generate random initial design with design points and the approximate allocation (For EW)

## Usage

```
EW_design_initial_self(
    k.continuous,
    factor.level,
    lvec,
    uvec,
    bvec_matrix,
    h.func,
    link = "continuation",
    EW_Fi.func = EW_Fi_MLM_func,
    delta = 1e-06,
    epsilon = 1e-12,
    maxit = 1000
)
```

## Arguments

k.continuous	number of continuous variables
factor.level	lower, upper limit of continuous variables, and discrete levels of categorical variables, continuous factors come first
lvec	lower limit of continuous variables
uvec	upper limit of continuous variables
<pre>bvec_matrix</pre>	the matrix of the bootstrap parameter values of beta
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" $$
EW_Fi.func	function, is used to calculate the Expectation of Fisher information for a design point - default to be EW_Fi_MLM_func() in the package
delta	tuning parameter, the distance threshold, $\  \mathbf{x}_{i}(0) - \mathbf{x}_{j}(0) \  \ge \text{delta}$
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 Fisher information matrix for the random initial design

#### **Examples**

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

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

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#### **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 cur-

rent design w/o new point

EU\_x matrix in the algorithm, get from EW\_Fi\_MLM\_func() function

link link multinomial link function, default is "continuation", other choices "base-

line", "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 Function to generate the Expectation of fisher information at one de-

sign point xi for multinomial logit models

## Description

Function to generate the Expectation of 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 bootstrap parameter values of beta

link multinomial logit model link function name "baseline", "cumulative", "adja-

cent", or "continuation", default to be "continuation"

#### Value

F\_x Fisher information matrix at x\_i

EU\_x U matrix for calculation the Expectation of Fisher information matrix at x\_i

#### **Examples**

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: . 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.

```
EW_ForLion_GLM_Optimal(
  n.factor,
  factor.level,
  hfunc,
  joint_Func_b,
  Lowerbounds,
  Upperbounds,
  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 al-

ways 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

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

link link function, default "logit", other links: "probit", "cloglog", "loglog", "cau-

chit", "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 func-

tion 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 EW lift-one with additional

"nram" number of random approximate allocation, default to be FALSE

nram when random == TRUE, the function will run EW lift-one nram number of

initial proportion p00, default is 3

logscale TRUE or FALSE, if TRUE then the EW ForLion will run EW lift-one with

logscale, which is EW\_liftoneDoptimal\_log\_GLM\_func(); if FALSE then For-Lion 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 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**

```
#Example Crystallography Experiment
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(4,-3)
paras_upperbound<-c(10,3)
gjoint_b<- function(x) {
Func_b<-1/(prod(paras_upperbound-paras_lowerbound))
  ##the prior distributions are follow uniform distribution
return(Func_b)
}
EW_ForLion_GLM_Optimal(n.factor=n.factor.temp, factor.level=factor.level.temp,
hfunc=hfunc.temp,joint_Func_b=gjoint_b, Lowerbounds=paras_lowerbound,
Upperbounds=paras_upperbound, link=link.temp, reltol=1e-2, rel.diff=0.01,
optim_grad=FALSE, maxit=500, random=FALSE, nram=3, logscale=FALSE, Xini=NULL)</pre>
```

EW\_ForLion\_MLM\_Optimal

EW ForLion function for multinomial logit models

## **Description**

EW ForLion function for multinomial logit models

```
EW_ForLion_MLM_Optimal(
  J,
  n.factor,
  factor.level,
  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
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
<pre>bvec_matrix</pre>	the matrix of the bootstrap 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 pints 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 EW lift-one with additional "nram" number of random approximate allocation, default to be FALSE
nram	when random $==$ TRUE, the function will run EW 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 func-
	tion 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){
matrix(data=c(0, 1, 2*y, 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 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,
         hfunc=hfunc.temp,h.prime=h.prime.temp, bvec_matrix=bvec_bootstrap,rel.diff=1,
         link=link.temp, optim_grad=FALSE)
```

```
EW_liftoneDoptimal_GLM_func
```

EW Lift-one algorithm for D-optimal approximate design

#### **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

Χ	Model matrix, with nrow = num of design points and ncol = num of parameters
E_w	$\label{lem:problem} Diagonal\ of\ E\_W\ matrix\ in\ Fisher\ information\ matrix,\ can\ be\ calculated\ EW\_Xw\_maineffects\_self()$ 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 Fisher information matrix of the reported EW D-optimal design

convergence Convergence TRUE or FALSE

itmax number of the iteration

```
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)</pre>
```

```
d2 \leftarrow stats::dnorm(x[2], mean = mu2, sd = sigma2)
d3 <- stats::dnorm(x[3], mean = mu3, sd = sigma3)
d4 \leftarrow stats::dnorm(x[4], mean = mu0, sd = sigma0)
return(d1 * d2 * d3 * d4)
\verb|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), ncol=3, by row=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) {
\label{temp} \verb| EW_Xw_maineffects_self(x=x.temp[i,],joint_Func_b=gjoint_b, Lowerbounds=paras_lowerbound, for the property of the property of
                                                                                  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)
```

 ${\tt EW\_liftoneDoptimal\_log\_GLM\_func}$ 

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**

Χ	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

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

```
hfunc.temp = function(y) \{c(y,1);\}; # y -> h(y)=(y1,y2,y3,1)
link.temp="logit"
paras_lowerbound<-rep(-Inf, 4)</pre>
paras_upperbound<-rep(Inf, 4)</pre>
gjoint_b<- function(x) {</pre>
mu1 <- -0.5; sigma1 <- 1
mu2 <- 0.5; sigma2 <- 1
mu3 <- 1; sigma3 <- 1
mu0 <- 1; sigma0 <- 1
d1 \leftarrow stats::dnorm(x[1], mean = mu1, sd = sigma1)
d2 \leftarrow stats::dnorm(x[2], mean = mu2, sd = sigma2)
d3 \leftarrow stats::dnorm(x[3], mean = mu3, sd = sigma3)
d4 \leftarrow 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,],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
р	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 bootstrap 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 $\frac{1}{2}$
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 Expectation of 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){
\texttt{matrix}(\texttt{data=c(1,y,y*y,0,0,0,0,0,1,y,0,0,0,0,0}), \ \texttt{nrow=3}, \ \texttt{ncol=5}, \ \texttt{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_liftoneDoptimal_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  $E_w=E(nu(beta^T h(x)))$  give a design point  $x=(1,x1,...,xd)^T$ 

#### **Description**

function for calculating X=h(x) and  $E_w=E(nu(beta^T h(x)))$  give a design point  $x=(1,x1,...,xd)^T$ 

```
EW_Xw_maineffects_self(
    x,
    joint_Func_b,
    Lowerbounds,
    Upperbounds,
    link = "logit",
```

Fi\_MLM\_func 19

```
h.func = NULL
)
```

#### **Arguments**

#### 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)</pre>
paras_upperbound<-rep(Inf, 4)</pre>
gjoint_b<- function(x) {</pre>
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)</pre>
d2 \leftarrow stats::dnorm(x[2], mean = mu2, sd = sigma2)
d3 <- stats::dnorm(x[3], mean = mu3, sd = sigma3)
d4 \leftarrow 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,joint_Func_b=gjoint_b, Lowerbounds=paras_lowerbound,
 Upperbounds=paras_upperbound, link=link.temp, h.func=hfunc.temp)
```

Fi\_MLM\_func

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

#### **Description**

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

#### Usage

```
Fi_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", "adja-

cent", 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"
Fi_MLM_func(X_x=X_x.temp, bvec=bvec.temp, link=link.temp)
```

ForLion\_GLM\_Optimal

ForLion for generalized linear models

## 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,
    hfunc,
    bvec,
    link,
    reltol = 1e-05,
    rel.diff = 0,
    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
bvec	assumed parameter values of model parameters beta, same length of $h(y)$
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
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 \rightarrow 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, hfunc=hfunc.temp, bvec=b.temp, link=link.temp, reltol=1e-2, rel.diff=0.03, maxit=500, random=FALSE, nram=3, logscale=TRUE)
```

ForLion\_MLM\_Optimal

ForLion function for multinomial logit models

#### 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.

```
ForLion_MLM_Optimal(
   J,
   n.factor,
   factor.level,
   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
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, $\parallel$ x_i(0) - x_j(0) $\parallel$ >= delta, default 1e-5
epsilon	for 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 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

```
m=5
p = 10
J=5
link.temp = "cumulative"
n.factor.temp = c(0,0,0,0,0,0,2) # 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, hfunc=hfunc.temp,
h.prime=h.prime.temp, bvec=bvec.temp, link=link.temp, optim_grad=FALSE)
```

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GLM\_Exact\_Design

Approximation to exact design algorithm for generalized linear model

## Description

Approximation to exact design algorithm for generalized linear model

## Usage

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

## Arguments

k.continuous	number of continuous factors
design_x	the matrix with rows indicating design point which we got from the approximate design
design_p	D-optimal approximate allocation
det.design	the determinant of D-optimal approximate allocation
р	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	assumed parameter values of model parameters beta, same length of $h(y)$
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
rel.diff	points with distance less than that will be merged
L	rounding factor

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 function, default "logit", other links: "probit", "cloglog", "loglog", "cauchit", "log", "identity"

#### Value

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

```
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) {</pre>
Func_b<-1/(prod(paras_upperbound-paras_lowerbound))</pre>
 ##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,joint_Func_b=gjoint_b,
 Lowerbounds=paras_lowerbound, Upperbounds=paras_upperbound, rel.diff=0,L=1,
 N=100, hfunc=hfunc.temp, link=link.temp)
```

```
{\tt 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**

Χ	Model matrix, with nrow = num of design points and ncol = num of parameters
W	$\label{lem:problem} Diagonal\ of\ W\ matrix\ in\ Fisher\ information\ matrix,\ can\ be\ calculated\ Xw\_maineffects\_self()$ 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$X;
w.vec[i]=htemp$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**

Χ	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 W	/hen random ==	TRUE, the	function wil	l 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-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$X;
w.vec[i]=htemp$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

```
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,

#### 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
```

default is 3

```
\begin{array}{l} 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"); \} \end{array}
```

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```
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)
liftoneDoptimal_MLM_func(m=m,p=p,Xi=Xi,J=J,thetavec=thetavec,
link="cumulative",p00=rep(1/5,5), random=FALSE)
```

MLM\_Exact\_Design

Approximation to exact design algorithm for multinomial logit model

## Description

Approximation to exact design algorithm for multinomial logit model

#### 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 D-optimal approximate allocation

det.design the determinant of D-optimal approximate allocation

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 bootstrap parameter values of beta

rel.diff points with distance less than that will be merged

L rounding factor

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 EW D-optimal or D-optimal exact allocation

rel.efficiency relative efficiency of the Exact and Approximate Designs

nu1\_cauchit\_self 33

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

Х

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**

Х

vector of eta, eta=X\*beta

#### Value

the first derivative of nu function given eta for identity link

nu1\_loglog\_self

#### **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**

Χ

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**

Χ

vector of eta, eta=X\*beta

nu1\_log\_self 35

#### 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**

Х

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

```
nu1_probit_self(x)
```

36 nu2\_cauchit\_self

#### **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

vector of eta, eta=X\*beta

#### Value

the second derivative of nu function for cauchit link

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

nu2\_identity\_self 37

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

Х

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**

Х

vector of eta, eta=X\*beta

#### Value

the second derivative of nu function for logit link

nu2\_log\_self

#### **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**

Х

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

Х

vector of eta, eta=X\*beta

nu2\_probit\_self 39

#### 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 = nu(eta) given eta for cauchit link

```
nu_cauchit_self(x)
```

40 nu\_identity\_self

#### **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 = nu(eta) given eta for identity link

## Usage

```
nu_identity_self(x)
```

#### **Arguments**

Χ

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

## Value

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

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

nu\_logit\_self 41

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**

Х

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 = nu(eta) given eta for loglog link

#### Usage

```
nu_loglog_self(x)
```

## Arguments

Χ

vector of eta, eta=X\*beta

#### Value

diagonal element of W matrix which is nu(eta)

nu\_probit\_self

#### **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 = nu(eta) given eta for log link

#### Usage

```
nu_log_self(x)
```

## Arguments

Х

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_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

Х

vector of eta, eta=X\*beta

print.design\_output 43

#### Value

diagonal element of W matrix which is nu(eta)

## **Examples**

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

print.design\_output

Print Method for Design Output from ForLion Algorithm

## **Description**

Custom print method for a list containing design information.

## Usage

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

## Arguments

x An object of class 'design\_output'.... Additional arguments (ignored).

#### Value

Invisibly returns 'x'.

 $print.list\_output$ 

Print Method for list\_output Objects

## Description

Custom print method for objects of class 'list\_output'.

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

svd\_inverse

#### **Arguments**

x An object of class 'list\_output'.

... Additional arguments (ignored).

#### Value

Invisibly returns 'x' (the input object).

svd\_inverse

SVD Inverse Of A Square Matrix 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.

## Description

SVD Inverse Of A Square Matrix 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**

x the matrix for calculation of inverse

#### Value

the inverse of the matrix x

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

45 xmat\_discrete\_self

xmat\_discrete\_self

Generate GLM random initial designs within ForLion algorithm

## **Description**

Generate GLM random initial designs within ForLion algorithm

## Usage

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

#### Arguments

xlist a list of factor levels within ForLion algorithm, for example, a binary factor

might be c(-1,1), a continuous factor within range of (25,45) will be c(25,45).

maximum number of rows of the design matrix rowmax

#### 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  $x=(x1,...,xd)^T$ 

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

#### **Arguments**

```
 \begin{array}{lll} 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" \\ \\ h. func & function h(x)=& (h1(x),...,hp(x)), default (1,x1,...,xd) \\ \end{array}
```

#### Value

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

```
# 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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