Package ‘SLSEdesign’

June 5, 2025

Title Optimal Regression Design under the Second-Order Least Squares Estimator

Version 0.0.5

Description With given inputs that include number of points, discrete design space, a measure of skewness, models and parameter value, this package calculates the objective value, optimal designs and plot the equivalence theory under A- and D-optimal criteria under the second-order Least squares estimator. This package is based on the paper ``Properties of optimal regression designs under the second-order least squares estimator'' by Chi-Kuang Yeh and Julie Zhou (2021) <doi:10.1007/s00362-018-01076-6>.

URL https://github.com/chikuang/SLSEdesign

BugReports https://github.com/chikuang/SLSEdesign/issues

License GPL-3

Encoding UTF-8

RoxygenNote 7.3.2

Imports CVXR

Suggests knitr, rmarkdown

VignetteBuilder knitr

NeedsCompilation no

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Repository CRAN

Date/Publication 2025-06-05 16:10:02 UTC

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`Aopt` *Calculate the A-optimal design under the second-order Least squares estimator*

Description

Calculate the A-optimal design under the second-order Least squares estimator

Usage

```
Aopt(N, u, tt, FUN, theta, num_iter = 1000)
```

Arguments

`N`	The number of sample points in the design space.
`u`	The discretized design space.
`tt`	The level of skewness between 0 to 1 (inclusive). When tt=0, it is equivalent to compute the A-optimal design under the ordinary least squares estimator.
`FUN`	The function to calculate the derivative of the given model.
`theta`	The parameter value of the model.
`num_iter`	Maximum number of iteration.

Details

This function calculates the A-optimal design and the loss function under the A-optimality. The loss function under A-optimality is defined as the trace of the inverse of the Fisher information matrix

Value

A list that contains 1. Value of the objective function at solution. 2. Status. 3. Optimal design

Examples

```
poly3 <- function(xi, theta){
  matrix(c(1, xi, xi^2, xi^3), ncol = 1)
}
Npt <- 101
my_design <- Aopt(N = Npt, u = seq(-1, +1, length.out = Npt),
   tt = 0, FUN = poly3, theta = rep(0,4), num_iter = 2000)
round(my_design$design, 3)
my_design$val
```

calc_phi *Calculate the loss function of the A-, c- or D-optimal design*

Description

Calculate the loss function of the A-, c- or D-optimal design

Usage

```
calc_phi(
  design,
  theta,
  FUN,
  tt,
  A,
  criterion = "D",
  cVec = rep(0, length(theta))
)
```

Arguments

design	The resulted design that contains the design points and the associated weights
theta	The parameter value of the model
FUN	The function to calculate the derivative of the given model.
tt	The level of skewness
A	The calculated covariance matrix
criterion	The criterion to be used for the design, either "D" for D-optimality or "A" for A-optimality. Default is "D".
cVec	c vector used to determine the combination of the parameters. This is only used in c-optimality

Details

This function calculates the loss function of the design problem under the A- or D-optimality. The loss functions under A-, or D-optimality are defined as the trace and log determinant of the inverse of the Fisher information matrix

Value

The loss of the model at each design points

Examples

```
my_design <- data.frame(location = c(0, 180), weight = c(1/2, 1/2))
theta <- c(0.05, 0.5)
peleg <- function(xi, theta){
   deno <- (theta[1] + xi * theta[2])^2
   rbind(-xi/deno, -xi^2/deno)
}
A <- matrix(c(1, 0, 0, 0, 0.2116, 1.3116, 0, 1.3116, 15.462521), byrow = TRUE, ncol = 3)
res <- calc_phi(my_design, theta, peleg, 0, A, criterion = "A")
res
```

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copt — *Calculate the c-optimal design under the SLSE with the given combination of the parameters*

Description

Calculate the c-optimal design under the SLSE with the given combination of the parameters

Usage

```
copt(N, u, tt, FUN, theta, num_iter = 1000, cVec)
```

Arguments

`N`	The number of sample points in the design space.
`u`	The discretized design space.
`tt`	The level of skewness. When tt=0, it is equivalent to compute the c-optimal design under the ordinary least squares estimator.
`FUN`	The function to calculate the derivative of the given model.
`theta`	The parameter value of the model.
`num_iter`	Maximum number of iteration.
`cVec`	c vector used to determine the combination of the parameters

Details

This function calculates the c-optimal design and the loss function under the c-optimality. The loss function under c-optimality is defined as the log determinant of the inverse of the Fisher information matrix.

Value

A list that contains 1. Value of the objective function at solution. 2. Status. 3. Optimal design

Examples

```
poly3 <- function(xi, theta){
  matrix(c(1, xi, xi^2, xi^3), ncol = 1)
}
Npt <- 101
my_design <- copt(N = Npt, u = seq(-1, +1, length.out = Npt),
   tt = 0, FUN = poly3, theta = rep(0,4), num_iter = 2000,
   cVec = c(0,1,1,1))
round(my_design$design, 3)
my_design$val
```

Dopt *Calculate the D-optimal design under the SLSE*

Description

Calculate the D-optimal design under the SLSE

Usage

```
Dopt(N, u, tt, FUN, theta, num_iter = 1000)
```

Arguments

N	The number of sample points in the design space.
u	The discretized design space.
tt	The level of skewness. When tt=0, it is equivalent to compute the D-optimal design under the ordinary least squares estimator.
FUN	The function to calculate the derivative of the given model.
theta	The parameter value of the model.
num_iter	Maximum number of iteration.

Details

This function calculates the D-optimal design and the loss function under the D-optimality. The loss function under D-optimality is defined as the log determinant of the inverse of the Fisher information matrix.

Value

A list that contains 1. Value of the objective function at solution. 2. Status. 3. Optimal design

Examples

```
poly3 <- function(xi, theta){
  matrix(c(1, xi, xi^2, xi^3), ncol = 1)
}
Npt <- 101
my_design <- Dopt(N = Npt, u = seq(-1, +1, length.out = Npt),
   tt = 0, FUN = poly3, theta = rep(0,4), num_iter = 2000)
round(my_design$design, 3)
my_design$val
```

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plot_dispersion — *Verify the optimality condition for an optimal design (A-, c- or D-optimality)*

Description

Verify the optimality condition for an optimal design (A-, c- or D-optimality)

Usage

```
plot_dispersion(
  u,
  design,
  tt,
  FUN,
  theta,
  criterion = "D",
  cVec = rep(0, length(theta))
)
```

Arguments

u	The discretized design points
design	The optimal design containing the design points and the associated weights
tt	The level of skewness
FUN	The function to calculate the derivative of the given model
theta	The parameter value of the model
criterion	The optimality criterion: one of "A", "c", or "D"
cVec	c vector used to determine the combination of the parameters. This is only used in c-optimality

Details

This function visualizes the directional derivative under A-, c-, or D-optimality using the general equivalence theorem. For an optimal design, the directional derivative should not exceed the reference threshold

Value

A plot verifying the general equivalence condition for the specified optimal design

Examples

```
poly3 <- function(xi, theta){
  matrix(c(1, xi, xi^2, xi^3), ncol = 1)
}
design_A <- data.frame(location = c(-1, -0.464, 0.464, 1),
                       weight = c(0.151, 0.349, 0.349, 0.151))
design_D = data.frame(location = c(-1, -0.447, 0.447, 1),
                      weight = rep(0.25, 4))
u <- seq(-1, 1, length.out = 201)
par(mfrow = c(2,2))
plot_dispersion(u, design_A, tt = 0, FUN = poly3, theta = rep(0, 4), criterion = "A")
plot_dispersion(u, design_A, tt = 0, FUN = poly3, theta = rep(0, 4), criterion = "D")

plot_dispersion(u, design_D, tt = 0, FUN = poly3, theta = rep(0, 4), criterion = "A")
plot_dispersion(u, design_D, tt = 0, FUN = poly3, theta = rep(0, 4), criterion = "D")
```

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plot_weight — *Plot the weight distribution of the optimal design for univaraite regression model*

Description

Plot the weight distribution of the optimal design for univaraite regression model

Usage

```
plot_weight(design)
```

Arguments

design	The resulted design that contains the design points and the associated weights

Details

This functions produce a figure that contains the location and their associated weights of the resulted optimal design measures.

Value

The plot that shows the given optimal design

Examples

```
Des = list(location = c(-1, +1), weight = c(0.5, 0.5))
plot_weight(Des)
```

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