Package 'SLSEdesign'

May 30, 2024

Title Optimal Regression Design under the Second-Order Least Squares

Estimator

Version 0.0.3
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="">.</doi:10.1007>
<pre>URL https://github.com/chikuang/SLSEdesign</pre>
BugReports https://github.com/chikuang/SLSEdesign/issues
License GPL-3
Encoding UTF-8
RoxygenNote 7.3.1
Imports CVXR
Suggests knitr, rmarkdown
VignetteBuilder knitr
NeedsCompilation no
Author Chi-Kuang Yeh [aut, cre] (https://orcid.org/0000-0001-7057-2096), Julie Zhou [aut, ctb], Jason Hou-Liu [ctb]
Maintainer Chi-Kuang Yeh <chi-kuang.yeh@uwaterloo.ca></chi-kuang.yeh@uwaterloo.ca>
Repository CRAN
Date/Publication 2024-05-29 23:30:08 UTC
R topics documented:
Aopt

2 Aopt

	Dopt plot_direction_Aopt plot_direction_Dopt							. 6
	plot_weight							
Index								9
Aopt		'alculate stimator	the A-o	ptima	ıl design	under the seco	ond-order Least squa	res

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

```
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</pre>
```

calc_phiA 3

calc_phiA Calculate the loss function of the A-optimal design

Description

Calculate the loss function of the A-optimal design

Usage

```
calc_phiA(design, theta, FUN, tt, A)
```

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
Α	The calculated covariance matrix

Details

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

Value

The loss of the model at each design points

```
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_phiA(my_design, theta, peleg, 0, A)
res</pre>
```

4 calc_phiD

calc		

Calculate the loss function of the D-optimal design

Description

Calculate the loss function of the D-optimal design

Usage

```
calc_phiD(design, theta, FUN, tt, A)
```

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
Α	The calculated covariance matrix

Details

This function calculates the loss function of the design problem 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

The loss of the model at each design points

```
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_phiA(my_design, theta, peleg, 0, A)
res</pre>
```

Dopt 5

п	\mathbf{a}	_	 _

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

```
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</pre>
```

6 plot_direction_Aopt

plot_direction_Aopt

Verify the optimality condition for the A-optimal design

Description

Verify the optimality condition for the A-optimal design

Usage

```
plot_direction_Aopt(u, design, tt, FUN, theta)
```

Arguments

u The discretized design points.

design The A-optimal design that contains 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.

Details

This function produces the figure for the directional derivative of the given A-optimal design of the compact supports. According to the general equivalence theorem, for an optimal design, all the negative value of the directional derivative should be below zero line.

Value

The plot of the negative value of the directional derivative of an A-optimal design

plot_direction_Dopt 7

plot_direction_Dopt

Verify the optimality condition for the D-optimal design

Description

Verify the optimality condition for the D-optimal design

Usage

```
plot_direction_Dopt(u, design, tt, FUN, theta)
```

Arguments

u	The discretized design points.
design	The D-optimal design that contains 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.

Details

This function produces the figure for the negative value of the directional derivative of the given D-optimal design of the compact supports. According to the general equivalence theorem, for an optimal design, all the directional derivative should be below zero line.

Value

The plot of the negative value of the directional derivative of a D-optimal design

```
poly3 <- function(xi, theta){
    matrix(c(1, xi, xi^2, xi^3), ncol = 1)
}
design = data.frame(location = c(-1, -0.447, 0.447, 1),
    weight = rep(0.25, 4))
u = seq(-1, 1, length.out = 201)
plot_direction_Dopt(u, design, tt=0, FUN = poly3,
    theta = rep(0, 4))</pre>
```

8 plot_weight

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

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

Index

```
Aopt, 2

calc_phiA, 3

calc_phiD, 4

Dopt, 5

plot_direction_Aopt, 6
plot_direction_Dopt, 7
plot_weight, 8
```