Package 'optedr'

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Title Calculating Optimal and D-Augmented Designs

Version 2.0.0

Description Calculates D-, Ds-, A- and I-optimal designs for non-linear models, via an implementation of the cocktail algorithm (Yu, 2011, <doi:10.1007/s11222-010-9183-2>). Compares designs via their efficiency, and D-augments any design with a controlled efficiency. An efficient rounding function has been provided to transform approximate designs to exact designs.

License GPL-3

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URL https://github.com/kezrael/optedr

BugReports https://github.com/kezrael/optedr/issues

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R **topics documented:**

add_design   *Add two designs*

Description

Add two designs

Usage

```
add_design(design_1, design_2, alpha)
```

Arguments

design_1   A dataframe with 'Point' and 'Weight' as columns that represent the first design to add

design_2   A dataframe with 'Point' and 'Weight' as columns that represent the second design to add

alpha   Weight of the first design

Value

A design as a dataframe with the weighted addition of the two designs

add_points   *Update design given crosspoints and alpha*

Description

Given a set of points, a weight and the design, the function adds these points to the new design with uniform weight, and combined weight alpha

Usage

```
add_points(points, alpha, design)
```

Arguments

points	Points to be added to the design
alpha	Combined weight of the new points to be added to the design
design	A design as a dataframe with "Point" and "Weight" columns

Value

A design as a dataframe with "Point" and "Weight" columns that is the addition of the design and the new points

---

augment_design	*Augment Design*

Description

Augments a design. The user gives an initial design for which he would like to add points and specifies the weight of the new points. Then he is prompted to choose a minimum efficiency. After that, the candidate points region is calculated and the user can choose the points and weights to add.

Usage

```
augment_design(
  criterion,
  init_design,
  alpha,
  model,
  parameters,
  par_values,
  design_space,
  calc_optimal_design,
  par_int = NA,
  matB = NA,
  distribution = NA,
  weight_fun = function(x) 1
)
```

Arguments

criterion character variable with the chosen optimality criterion. Can be one of the following:

- 'D-Optimality'
- 'Ds-Optimality'
- 'A-Optimality'
- 'I-Optimality'

init_design	dataframe with "Point" and "Weight" columns that represents the initial design to augment
alpha	combined weight of the new points
model	formula that represents the model with x as the independent variable
parameters	character vector with the unknown parameters of the model to estimate
par_values	numeric vector with the initial values of the unknown parameters
design_space	numeric vector with the limits of the space of the design
calc_optimal_design	
	boolean parameter, if TRUE, the optimal design is calculated and efficiencies of the initial and augmented design are given
par_int	optional numeric vector with the index of the `parameters` of interest for Ds-optimality.
matB	optional matrix of dimensions k x k, integral of the information matrix of the model over the interest region for I-optimality.
distribution	character specifying the probability distribution of the response. Can be one of the following:

- 'Homoscedasticity'
- 'Gamma', which can be used for exponential or normal heteroscedastic with constant relative error
- 'Poisson'
- 'Logistic'
- 'Log-Normal' (work in progress)

weight_fun	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A dataframe that represents the D-augmented design

Examples

```
init_des <- data.frame("Point" = c(30, 60, 90), "Weight" = c(1/3, 1/3, 1/3))
augment_design("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), TRUE)
augment_design("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), FALSE)
```

---

check_inputs *Check Inputs*

Description

Function to check that the inputs given to the function opt_des are correct. If not, throws the correspondent error message.

Usage

```
check_inputs(
  Criterion,
  model,
  parameters,
  par_values,
  design_space,
  init_design,
  join_thresh,
  delete_thresh,
  delta,
  tol,
  tol2,
  par_int,
  matB,
  reg_int,
  desired_output,
  weight_fun
)
```

Arguments

Criterion	character variable with the chosen optimality criterion. Can be one of the following:
	• 'D-Optimality'
	• 'Ds-Optimality'
	• 'A-Optimality'
	• 'I-Optimality'
model	formula describing the model to calculate the optimal design. Must use x as the variable.
parameters	character vector with the parameters of the models, as written in the formula.
par_values	numeric vector with the parameters nominal values, in the same order as given in parameters.
design_space	numeric vector with the limits of the space of the design.
init_design	optional dataframe with the initial design for the algorithm. A dataframe with two columns:

- Point contains the support points of the design.
- Weight contains the corresponding weights of the Points.

join_thresh	optional numeric value that states how close, in real units, two points must be in order to be joined together by the join heuristic.
delete_thresh	optional numeric value with the minimum weight, over 1 total, that a point needs to have in order to not be deleted from the design.
delta	optional numeric value in (0, 1), parameter of the algorithm.
tol	optional numeric value for the convergence of the weight optimizing algorithm.
tol2	optional numeric value for the stop criterion: difference between maximum of sensitivity function and optimality criterion.
par_int	optional numeric vector with the index of the parameters of interest for Ds-optimality.
matB	optional matrix of dimensions k x k, integral of the information matrix of the model over the interest region for I-optimality.
reg_int	optional numeric vector of two components with the bounds of the interest region for I-Optimality.
desired_output	not functional yet: decide which kind of output you want.
weight_fun	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

---

crit	*Master function for the criterion function*

Description

Depending on the Criterion input, the function returns the output of the corresponding criterion function given the information matrix.

Usage

```
crit(Criterion, M, k = 0, par_int = c(1), matB = NA)
```

Arguments

Criterion	character variable with the chosen optimality criterion. Can be one of the following:
	'D-Optimality' 'Ds-Optimality' 'A-Optimality' 'I-Optimality'
M	information matrix for which the criterion value wants to be calculated.
k	numeric variable with the number of parameters of the model. Taken from the number of rows of the matrix if omitted.

par_int	numeric vector with the index of the parameters of interest of the model. Only for "Ds-Optimality".
matB	matrix of the integral of the information matrix over the interest region. Only for "I-Optimality".

Value

Numeric value of the optimality criterion for the information matrix.

---

crosspoints   *Calculate crosspoints*

Description

Given the parameters for augmenting a design, this function calculates the crosspoints in the efficiency function that delimit the candidate points region

Usage

```
crosspoints(val, sens, gridlength, tol, xmin, xmax)
```

Arguments

val	Efficiency value to solve in the curve relationing the space of the design and efficiency of new design
sens	Sensitivity function of the design for the model
gridlength	Number of points in the grid to find the crosspoints
tol	Tolerance that establishes how close two points close to one another are considered the same
xmin	Minimum of the space of the design
xmax	Maximum of the space of the design

Value

A numeric vector of crosspoints that define the candidate points region

daugment_design *D-Augment Design*

Description

D-Augments a design. The user gives an initial design for which he would like to add points and specifies the weight of the new points. Then he is prompted to choose a minimum efficiency. After that, the candidate points region is calculated and the user can choose the points and weights to add.

Usage

```
daugment_design(
  init_design,
  alpha,
  model,
  parameters,
  par_values,
  design_space,
  calc_optimal_design,
  weight_fun = function(x) 1
)
```

Arguments

init_design	dataframe with "Point" and "Weight" columns that represents the initial design to augment
alpha	combined weight of the new points
model	formula that represents the model with x as the independent variable
parameters	character vector with the unknown parameters of the model to estimate
par_values	numeric vector with the initial values of the unknown parameters
design_space	numeric vector with the limits of the space of the design
calc_optimal_design	
	boolean parameter, if TRUE, the optimal design is calculated and efficiencies of the initial and augmented design are given
weight_fun	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A dataframe that represents the D-augmented design

See Also

Other augment designs: dsaugment_design(), laugment_design()

Examples

```
init_des <- data.frame("Point" = c(30, 60, 90), "Weight" = c(1/3, 1/3, 1/3))
augment_design("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), TRUE)
augment_design("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), FALSE)
```

---

dcrit   *Criterion function for D-Optimality*

Description

Calculates the value of the D-Optimality criterion function, which follows the expression:

$$\phi_D = \left(\frac{1}{|M|}\right)^{1/k}$$

Usage

```
dcrit(M, k)
```

Arguments

M	information matrix for which the criterion value wants to be calculated.
k	numeric variable with the number of parameters of the model. Taken from the number of rows of the matrix if omitted.

Value

numeric value of the D-optimality criterion for the information matrix.

---

delete_points   *Remove low weight points*

Description

Removes the points of a design with a weight lower than a threshold, `delta`, and distributes that weights proportionally to the rest of the points.

Usage

```
delete_points(design, delta)
```

Arguments

design	The design from which to remove points as a dataframe with two columns:

- Point contains the support points of the design.
- Weight contains the corresponding weights of the Points.

delta	The threshold from which the points with such a weight or lower will be removed.

Value

The design without the removed points.

---

design_efficiency *Efficiency between optimal design and a user given design*

Description

Takes an optimal design provided from the function opt_des and a user given design and compares their efficiency

Usage

```
design_efficiency(opt_des_obj, design)
```

Arguments

opt_des_obj	an object given by the function opt_des.
design	dataframe that represents the design. Must have two columns:

- Point contains the support points of the design.
- Weight contains the corresponding weights of the Points.

Value

The efficiency as a value between 0 and 1

See Also

opt_des

Examples

```
result <- opt_des("D-Optimality", y ~ a * exp(-b / x), c("a", "b"), c(1, 1500), c(212, 422))
design <- data.frame("Point" = c(220, 240, 400), "Weight" = c(1 / 3, 1 / 3, 1 / 3))
design_efficiency(result, design)
```

---

dsaugment_design   *Ds-Augment Design*

Description

Ds-Augments a design. The user gives an initial design for which he would like to add points and specifies the weight of the new points. Then he is prompted to choose a minimum efficiency. After that, the candidate points region is calculated and the user can choose the points and weights to add.

Usage

```
dsaugment_design(
  init_design,
  alpha,
  model,
  parameters,
  par_values,
  par_int,
  design_space,
  calc_optimal_design,
  weight_fun = function(x) 1
)
```

Arguments

init_design	dataframe with "Point" and "Weight" columns that represents the initial design to augment
alpha	combined weight of the new points
model	formula that represents the model with x as the independent variable
parameters	character vector with the unknown parameters of the model to estimate
par_values	numeric vector with the initial values of the unknown parameters
par_int	optional numeric vector with the index of the parameters of interest for Ds-optimality.
design_space	numeric vector with the limits of the space of the design
calc_optimal_design	
	boolean parameter, if TRUE, the optimal design is calculated and efficiencies of the initial and augmented design are given
weight_fun	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A dataframe that represents the Ds-augmented design

See Also

Other augment designs: daugment_design(), laugment_design()

Examples

```
init_des <- data.frame("Point" = c(30, 60, 90), "Weight" = c(1/3, 1/3, 1/3))
augment_design("Ds-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), par_int = c(1), TRUE)
augment_design("Ds-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), par_int = c(1), FALSE)
```

---

dscrit *Criterion function for Ds-Optimality*

Description

Calculates the value of the Ds-Optimality criterion function, which follows the expression:

$$\phi_{Ds} = \left(\frac{|M_{22}|}{|M|} \right)^{1/s}$$

Usage

```
dscrit(M, par_int)
```

Arguments

M	information matrix for which the criterion value wants to be calculated.
par_int	numeric vector with the index of the parameters of interest of the model.

Value

Numeric value of the Ds-optimality criterion for the information matrix.

dsens   *Sensitivity function for D-Optimality*

Description

Calculates the sensitivity function from the gradient vector and the Identity Matrix.

Usage

```
dsens(grad, M)
```

Arguments

grad   A function in a single variable that returns the partial derivatives vector of the
                model.

M   Information Matrix for the sensitivity function.

Value

The sensitivity function as a matrix of single variable.

dssens   *Sensitivity function for Ds-Optimality*

Description

Calculates the sensitivity function from the gradient vector, the Identity Matrix and the parameters
of interest.

Usage

```
dssens(grad, M, par_int)
```

Arguments

grad   A function in a single variable that returns the partial derivatives vector of the
                model.

M   Information Matrix for the sensitivity function.

par_int   Numeric vector of the indexes of the parameters of interest for Ds-Optimality.

Value

The sensitivity function as a matrix of single variable.

DsWFMult   *Cocktail Algorithm implementation for Ds-Optimality*

Description

Function that calculates the Ds-Optimal designs for the interest parameters given by intPar. The rest of the parameters can help the convergence of the algorithm.

Usage

```
DsWFMult(
  init_design,
  grad,
  par_int,
  min,
  max,
  grid.length,
  join_thresh,
  delete_thresh,
  delta_weights,
  tol,
  tol2
)
```

Arguments

init_design	optional dataframe with the initial design for the algorithm. A dataframe with two columns:
	• Point contains the support points of the design.
	• Weight contains the corresponding weights of the Points.
grad	function of partial derivatives of the model.
par_int	numeric vector with the index of the parameters of interest. Only necessary when the Criterion chosen is 'Ds-Optimality'.
min	numeric value with the inferior bound of the space of the design.
max	numeric value with the upper bound of the space of the design.
grid.length	numeric value that gives the grid to evaluate the sensitivity function when looking for a maximum.
join_thresh	numeric value that states how close, in real units, two points must be in order to be joined together by the join heuristic.
delete_thresh	numeric value with the minimum weight, over 1 total, that a point needs to have in order to not be deleted from the design.
delta_weights	numeric value in (0, 1), parameter of the algorithm.
tol	numeric value for the convergence of the weight optimizing algorithm.
tol2	numeric value for the stop condition of the algorithm.

Value

list correspondent to the output of the correspondent algorithm called, dependent on the criterion. A list of two objects:

- optdes: a dataframe with the optimal design in two columns, `Point` and `Weight`.
- sens: a plot with the sensitivity function to check for optimality of the design.

See Also

Other cocktail algorithms: `DWFMult()`, `IWFMult()`, `WFMult()`

DWFMult *Cocktail Algorithm implementation for D-Optimality*

Description

Function that calculates the DsOptimal design. The rest of the parameters can help the convergence of the algorithm.

Usage

```
DWFMult(
  init_design,
  grad,
  min,
  max,
  grid.length,
  join_thresh,
  delete_thresh,
  k,
  delta_weights,
  tol,
  tol2
)
```

Arguments

init_design   optional dataframe with the initial design for the algorithm. A dataframe with two columns:

- `Point` contains the support points of the design.
- `Weight` contains the corresponding weights of the `Points`.

grad   function of partial derivatives of the model.

min   numeric value with the inferior bound of the space of the design.

max   numeric value with the upper bound of the space of the design.

grid.length	numeric value that gives the grid to evaluate the sensitivity function when looking for a maximum.
join_thresh	numeric value that states how close, in real units, two points must be in order to be joined together by the join heuristic.
delete_thresh	numeric value with the minimum weight, over 1 total, that a point needs to have in order to not be deleted from the design.
k	number of unknown parameters of the model.
delta_weights	numeric value in (0, 1), parameter of the algorithm.
tol	numeric value for the convergence of the weight optimizing algorithm.
tol2	numeric value for the stop condition of the algorithm.

Value

list correspondent to the output of the correspondent algorithm called, dependent on the criterion. A list of two objects:

- optdes: a dataframe with the optimal design in two columns, Point and Weight.
- sens: a plot with the sensitivity function to check for optimality of the design.

See Also

Other cocktail algorithms: DsWFMult(), IWFMult(), WFMult()

---

eff   *Efficiency between two Information Matrices*

Description

Efficiency between two Information Matrices

Usage

```
eff(Criterion, mat1, mat2, k = 0, intPars = c(1), matB = NA)
```

Arguments

Criterion	character variable with the chosen optimality criterion. Can be one of the following:
	• 'D-Optimality'
	• 'Ds-Optimality'
	• 'A-Optimality'
	• 'I-Optimality'
mat1	first information matrix, for the numerator.
mat2	second information matrix, for the denominator.

k	number of parameters of the model. Taken from the number of rows of the matrix if omitted.
intPars	numeric vector with the index of the parameters of interest of the model. Only for "Ds-Optimality".
matB	matrix of the integral of the information matrix over the interest region. Only for "I-Optimality".

Value

Efficiency of first design with respect to the second design, as a decimal number.

---

efficient_round	*Efficient Round*

Description

Takes an approximate design, and a number of points and converts the design to an approximate design. It uses the multiplier (n - l/2) and evens the total number of observations afterwards.

Usage

```
efficient_round(design, n, tol = 1e-05)
```

Arguments

design	a dataframe with columns "Point" and "Weight" that represents a design
n	an integer that represents the desired number of observations of the exact design
tol	optional parameter for the consideration of an integer in the rounding process

Value

a data.frame with columns "Point" and "Weight" representing an exact design with n observations

Examples

```
design_test <- data.frame("Point" = seq(1, 5, length.out = 7),
         "Weight" = c(0.1, 0.0001, 0.2, 0.134, 0.073, 0.2111, 0.2818))

efficient_round(design_test, 20)

exact_design <- efficient_round(design_test, 21)
aprox_design <- exact_design
aprox_design$Weight <- aprox_design$Weight/sum(aprox_design$Weight)
```

---

findmax   *Find Maximum*

Description

Searches the maximum of a function over a grid on a given interval.

Usage

```
findmax(sens, min, max, grid.length)
```

Arguments

sens	A single variable numeric function to evaluate.
min	Minimum value of the search interval.
max	Maximum value of the search interval.
grid.length	Length of the search interval.

Value

The value at which the maximum is obtained

---

findmaxval   *Find Maximum Value*

Description

Searches the maximum of a function over a grid on a given interval.

Usage

```
findmaxval(sens, min, max, grid.length)
```

Arguments

sens	A single variable numeric function to evaluate.
min	Minimum value of the search interval.
max	Maximum value of the search interval.
grid.length	Length of the search interval.

Value

The value of the maximum

---

findminval   *Find Minimum Value*

Description

Searches the maximum of a function over a grid on a given grid.

Usage

```
findminval(sens, min, max, grid.length)
```

Arguments

sens	a single variable numeric function to evaluate.
min	minimum value of the search grid.
max	maximum value of the search grid.
grid.length	length of the search grid.

Value

The value of the minimum

---

getCross2   *Give effective limits to candidate points region*

Description

Given the start of the candidates points region, the parity of the crosspoints and the boundaries of the space of the design returns the effective limits of the candidate points region. Those points, taken in pairs from the first to the last delimit the region.

Usage

```
getCross2(cross, min, max, start, par)
```

Arguments

cross	Vector of crosspoints in the sensitivity function given an efficiency and weight
min	Minimum of the space of the design
max	Maximum of the space of the design
start	Boolean that gives the effective start of the candidate points region
par	Boolean with the parity of the region

Value

Vector of effective limits of the candidate points region. Taken in pairs from the beginning delimit the region.

`getPar`   *Parity of the crosspoints*

Description

Determines if the number of crosspoints is even or odd given the vector of crosspoints

Usage

```
getPar(cross)
```

Arguments

cross   Vector of crosspoints in the sensitivity function given an efficiency and weight

Value

True if the number of crosspoints is even, false otherwise

`getStart`   *Find where the candidate points region starts*

Description

Given the crosspoints and the sensitivity function, this function finds where the candidate points region starts, either on the extreme of the space of the design or the first crosspoints

Usage

```
getStart(cross, min, max, val, sens_opt)
```

Arguments

cross   Vector of crosspoints in the sensitivity function given an efficiency and weight

min   Minimum of the space of the design

max   Maximum of the space of the design

val   Value of the sensitivity function at the crosspoints

sens_opt   Sensitivity function

Value

True if the candidate points region starts on the minimum, False otherwise

---

get_augment_region   *Get Augment Regions*

Description

Given a model and criterion, calculates the candidate points region. The user gives an initial design for which he would like to add points and specifies the weight of the new points. Then he is prompted to choose a minimum efficiency. After that, the candidate points region is calculated.

Usage

```
get_augment_region(
  criterion,
  init_design,
  alpha,
  model,
  parameters,
  par_values,
  design_space,
  calc_optimal_design,
  par_int = NA,
  matB = NA,
  distribution = NA,
  weight_fun = function(x) 1
)
```

Arguments

criterion   character with the chosen optimality criterion. Can be one of the following:

- 'D-Optimality'
- 'Ds-Optimality'
- 'A-Optimality'
- 'I-Optimality'

init_design   dataframe with "Point" and "Weight" columns that represents the initial design to augment

alpha   combined weight of the new points

model   formula that represent the model with x as the independent variable

parameters   character vector with the unknown parameters of the model to estimate

par_values   numeric vector with the initial values of the unknown parameters

design_space   numeric vector with the limits of the space of the design

calc_optimal_design

                  boolean parameter, if TRUE, the optimal design is calculated and efficiencies of the initial and augmented design are given

par_int	optional numeric vector with the index of the parameters of interest for Ds-optimality.
matB	optional matrix of dimensions k x k, integral of the information matrix of the model over the interest region for I-optimality.
distribution	character specifying the probability distribution of the response. Can be one of the following:

- 'Homoscedasticity'
- 'Gamma', which can be used for exponential or normal heteroscedastic with constant relative error
- 'Poisson'
- 'Logistic'
- 'Log-Normal' (work in progress)

weight_fun	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A vector of the points limiting the candidate points region

Examples

```
init_des <- data.frame("Point" = c(30, 60, 90), "Weight" = c(1/3, 1/3, 1/3))
get_augment_region("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), TRUE)
get_augment_region("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), FALSE)
```

---

get_daugment_region   *Get D-augment region*

Description

Given a model, calculates the candidate points region for D-Optimality. The user gives an initial design for which he would like to add points and specifies the weight of the new points. Then he is prompted to choose a minimum efficiency. After that, the candidate points region is calculated.

Usage

```
get_daugment_region(
  init_design,
  alpha,
  model,
  parameters,
  par_values,
  design_space,
  calc_optimal_design,
  weight_fun = function(x) 1
)
```

Arguments

`init_design`	dataframe with "Point" and "Weight" columns that represents the initial design to augment
`alpha`	combined weight of the new points
`model`	formula that represent the model with x as the independent variable
`parameters`	character vector with the unknown parameters of the model to estimate
`par_values`	numeric vector with the initial values of the unknown parameters
`design_space`	numeric vector with the limits of the space of the design
`calc_optimal_design`	
	boolean parameter, if TRUE, the optimal design is calculated and efficiencies of the initial and augmented design are given
`weight_fun`	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A vector of the points limiting the candidate points region

Examples

```
init_des <- data.frame("Point" = c(30, 60, 90), "Weight" = c(1/3, 1/3, 1/3))
get_augment_region("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), TRUE)
get_augment_region("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), FALSE)
```

  `get_dsaugment_region`   *Get Ds-augment region*

Description

Given a model, calculates the candidate points region for Ds-Optimality. The user gives an initial design for which he would like to add points and specifies the weight of the new points. Then he is prompted to choose a minimum efficiency. After that, the candidate points region is calculated.

Usage

```
get_dsaugment_region(
  init_design,
  alpha,
  model,
  parameters,
  par_values,
  par_int,
  design_space,
  calc_optimal_design,
  weight_fun = function(x) 1
)
```

Arguments

`init_design`	dataframe with "Point" and "Weight" columns that represents the initial design to augment
`alpha`	combined weight of the new points
`model`	formula that represent the model with x as the independent variable
`parameters`	character vector with the unknown parameters of the model to estimate
`par_values`	numeric vector with the initial values of the unknown parameters
`par_int`	optional numeric vector with the index of the `parameters` of interest for Ds-optimality.
`design_space`	numeric vector with the limits of the space of the design
`calc_optimal_design`	
	boolean parameter, if TRUE, the optimal design is calculated and efficiencies of the initial and augmented design are given
`weight_fun`	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A vector of the points limiting the candidate points region

See Also

Other augment region: [get_laugment_region()](get_laugment_region)

Examples

```
init_des <- data.frame("Point" = c(30, 60, 90), "Weight" = c(1/3, 1/3, 1/3))
get_augment_region("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), TRUE)
get_augment_region("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), FALSE)
```

`get_laugment_region`	*Get L-augment region*

Description

Given a model, calculates the candidate points region for L-Optimality. The user gives an initial design for which he would like to add points and specifies the weight of the new points. Then he is prompted to choose a minimum efficiency. After that, the candidate points region is calculated.

Usage

```
get_laugment_region(
  init_design,
  alpha,
  model,
  parameters,
  par_values,
  design_space,
  calc_optimal_design,
  matB,
  weight_fun = function(x) 1
)
```

Arguments

`init_design`	dataframe with "Point" and "Weight" columns that represents the initial design to augment
`alpha`	combined weight of the new points
`model`	formula that represent the model with x as the independent variable
`parameters`	character vector with the unknown parameters of the model to estimate
`par_values`	numeric vector with the initial values of the unknown parameters
`design_space`	numeric vector with the limits of the space of the design
`calc_optimal_design`	
	boolean parameter, if TRUE, the optimal design is calculated and efficiencies of the initial and augmented design are given
`matB`	optional matrix of dimensions k x k, integral of the information matrix of the model over the interest region for I-optimality.
`weight_fun`	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A vector of the points limiting the candidate points region

See Also

Other augment region: [`get_dsaugment_region()`](get_dsaugment_region)

Examples

```
init_des <- data.frame("Point" = c(30, 60, 90), "Weight" = c(1/3, 1/3, 1/3))
get_augment_region("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131, 1730.63, 233.426), c(1, 100), TRUE)
get_augment_region("D-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131, 1730.63, 233.426), c(1, 100), FALSE)
```

---

gradient	*Gradient function*

Description

Calculates the gradient function of a model with respect to the parameters, char_vars, evaluates it at the provided values and returns the result as a function of the variable x.

Usage

```
gradient(model, char_vars, values, weight_fun = function(x) 1)
```

Arguments

model	formula describing the model, which must contain only x, the parameters defined in char_vars and the numerical operators.
char_vars	character vector of the parameters of the model.
values	numeric vector with the nominal values of the parameters in char_vars.
weight_fun	optional function variable that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A function depending on x that's the gradient of the model with respect to char_vars

---

gradient22	*Gradient function for a subset of variables*

Description

Calculates the gradient function of a model with respect to a subset of the parameters given in par_int, char_vars, evaluates it at the provided values and returns the result as a function of the variable x.

Usage

```
gradient22(model, char_vars, values, par_int, weight_fun = function(x) 1)
```

Arguments

`model`	formula describing the model, which must contain only x, the parameters defined in `char_vars` and the numerical operators.
`char_vars`	character vector of the parameters of the model.
`values`	numeric vector with the nominal values of the parameters in `char_vars`.
`par_int`	vector of indexes indicating the subset of variables to omit in the calculation of the gradient.
`weight_fun`	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A function depending on x that's the gradient of the `model` with respect to `char_vars`

---

icrit	*Criterion function for I-Optimality*

Description

Calculates the value of the I-Optimality criterion function, which follows the expression:

$$\phi_I = Tr(M^{-1} \cdot B)$$

Usage

```
icrit(M, matB)
```

Arguments

`M`	information matrix for which the criterion value wants to be calculated.
`matB`	matrix of the integral of the information matrix over the interest region. Identity matrix for A-Optimality.

Value

Numeric value of the I-optimality criterion for the information matrix.

---

inf_mat *Information Matrix*

Description

Given the gradient vector of a model in a single variable model and a design, calculates the information matrix.

Usage

```
inf_mat(grad, design)
```

Arguments

grad
: A function in a single variable that returns the partial derivatives vector of the model.

design
: A dataframe that represents the design. Must have two columns:
    - Point contains the support points of the design.
    - Weight contains the corresponding weights of the Points.

Value

The information matrix of the design, a $k \times k$ matrix where k is the length of the gradient.

---

integrate_reg_int *Integrate IM*

Description

Integrates the information matrix over the region of interest to calculate matrix B to be used in I-Optimality calculation.

Usage

```
integrate_reg_int(grad, k, reg_int)
```

Arguments

grad
: function of partial derivatives of the model.

k
: number of unknown parameters of the model.

reg_int
: optional numeric vector of two components with the bounds of the interest region for I-Optimality.

Value

The integrated information matrix.

---

isens *Sensitivity function for I-Optimality*

Description

Calculates the sensitivity function from the gradient vector, the Information Matrix and the integral of the one-point Identity Matrix over the interest region. If instead the identity matrix is used, it can be used for A-Optimality.

Usage

```
isens(grad, M, matB)
```

Arguments

grad	A function in a single variable that returns the partial derivatives vector of the model.
M	Information Matrix for the sensitivity function.
matB	Matrix resulting from the integration of the one-point Information Matrix along the interest region.

Value

The sensitivity function as a matrix of single variable.

IWFMult *Cocktail Algorithm implementation for I-Optimality and A-Optimality (with matB = diag(k))*

Description

Function that calculates the I-Optimal designs given the matrix B (should be integral of the information matrix over the interest region), or A-Optimal if given diag(k). The rest of the parameters can help the convergence of the algorithm.

Usage

```
IWFMult(
  init_design,
  grad,
  matB,
  min,
  max,
  grid.length,
  join_thresh,
```

```
    delete_thresh,
    delta_weights,
    tol,
    tol2
)
```

Arguments

init_design   optional dataframe with the initial design for the algorithm. A dataframe with
                   two columns:

                        • Point contains the support points of the design.
                        • Weight contains the corresponding weights of the Points.

grad   function of partial derivatives of the model.

matB   optional matrix of dimensions k x k, integral of the information matrix of the
                   model over the interest region for I-optimality.

min   numeric value with the inferior bound of the space of the design.

max   numeric value with the upper bound of the space of the design.

grid.length   numeric value that gives the grid to evaluate the sensitivity function when look-
                   ing for a maximum.

join_thresh   numeric value that states how close, in real units, two points must be in order to
                   be joined together by the join heuristic.

delete_thresh   numeric value with the minimum weight, over 1 total, that a point needs to have
                   in order to not be deleted from the design.

delta_weights   numeric value in (0, 1), parameter of the algorithm.

tol   numeric value for the convergence of the weight optimizing algorithm.

tol2   numeric value for the stop condition of the algorithm.

Value

list correspondent to the output of the correspondent algorithm called, dependent on the criterion.
A list of two objects:

   • optdes: a dataframe with the optimal design in two columns, Point and Weight.

   • sens: a plot with the sensitivity function to check for optimality of the design.

See Also

Other cocktail algorithms: DWFMult(), DsWFMult(), WFMult()

---

laugment_design *L-Augment Design*

Description

L-Augments a design. The user gives an initial design for which he would like to add points and specifies the weight of the new points. Then he is prompted to choose a minimum efficiency. After that, the candidate points region is calculated and the user can choose the points and weights to add.

Usage

```
laugment_design(
  init_design,
  alpha,
  model,
  parameters,
  par_values,
  design_space,
  calc_optimal_design,
  matB,
  weight_fun = function(x) 1
)
```

Arguments

init_design	dataframe with "Point" and "Weight" columns that represents the initial design to augment
alpha	combined weight of the new points
model	formula that represents the model with x as the independent variable
parameters	character vector with the unknown parameters of the model to estimate
par_values	numeric vector with the initial values of the unknown parameters
design_space	numeric vector with the limits of the space of the design
calc_optimal_design	
	boolean parameter, if TRUE, the optimal design is calculated and efficiencies of the initial and augmented design are given
matB	optional matrix of dimensions k x k, integral of the information matrix of the model over the interest region for I-optimality.
weight_fun	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

A dataframe that represents the L-augmented design

See Also

Other augment designs: daugment_design(), dsaugment_design()

Examples

```
init_des <- data.frame("Point" = c(30, 60, 90), "Weight" = c(1/3, 1/3, 1/3))
augment_design("I-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), TRUE)
augment_design("I-Optimality", init_des, 0.25, y ~ 10^(a-b/(c+x)), c("a","b","c"),
  c(8.07131,  1730.63, 233.426), c(1, 100), FALSE)
```

---

opt_des   *Calculates the optimal design for a specified Criterion*

Description

The opt_des function calculates the optimal design for an optimality Criterion and a model input from the user. The parameters allows for the user to customize the parameters for the cocktail algorithm in case the default set does not provide a satisfactory output. Depending on the criterion, additional details are necessary. For 'Ds-Optimality' the par_int parameter is necessary. For 'I-Optimality' either the matB or reg_int must be provided.

Usage

```
opt_des(
  Criterion,
  model,
  parameters,
  par_values = c(1),
  design_space,
  init_design = NULL,
  join_thresh = -1,
  delete_thresh = 0.02,
  delta = 1/2,
  tol = 1e-05,
  tol2 = 1e-05,
  par_int = NULL,
  matB = NULL,
  reg_int = NULL,
  desired_output = c(1, 2),
  distribution = NA,
  weight_fun = function(x) 1
)
```

Arguments

`Criterion`	character variable with the chosen optimality criterion. Can be one of the following:

- 'D-Optimality'
- 'Ds-Optimality'
- 'A-Optimality'
- 'I-Optimality'

`model`	formula describing the model to calculate the optimal design. Must use x as the variable.
`parameters`	character vector with the parameters of the models, as written in the `formula`.
`par_values`	numeric vector with the parameters nominal values, in the same order as given in `parameters`.
`design_space`	numeric vector with the limits of the space of the design.
`init_design`	optional dataframe with the initial design for the algorithm. A dataframe with two columns:

- `Point` contains the support points of the design.
- `Weight` contains the corresponding weights of the `Points`.

`join_thresh`	optional numeric value that states how close, in real units, two points must be in order to be joined together by the join heuristic.
`delete_thresh`	optional numeric value with the minimum weight, over 1 total, that a point needs to have in order to not be deleted from the design.
`delta`	optional numeric value in (0, 1), parameter of the algorithm.
`tol`	optional numeric value for the convergence of the weight optimizing algorithm.
`tol2`	optional numeric value for the stop criterion: difference between maximum of sensitivity function and optimality criterion.
`par_int`	optional numeric vector with the index of the `parameters` of interest for Ds-optimality.
`matB`	optional matrix of dimensions k x k, integral of the information matrix of the model over the interest region for I-optimality.
`reg_int`	optional numeric vector of two components with the bounds of the interest region for I-Optimality.
`desired_output`	not functional yet: decide which kind of output you want.
`distribution`	character variable specifying the probability distribution of the response. Can be one of the following:

- 'Homoscedasticity'
- 'Gamma', which can be used for exponential or normal heteroscedastic with constant relative error
- 'Poisson'
- 'Logistic'
- 'Log-Normal' (work in progress)

`weight_fun`	optional one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response

Value

a list of two objects:

- optdes: a dataframe with the optimal design in two columns, `Point` and `Weight`.
- sens: a plot with the sensitivity function to check for optimality of the design.

Examples

```
opt_des("D-Optimality", y ~ a * exp(-b / x), c("a", "b"), c(1, 1500), c(212, 422))
```

---

plot.optdes   *Plot function for optdes*

Description

Plot function for optdes

Usage

```
## S3 method for class 'optdes'
plot(x, ...)
```

Arguments

x	An object of class optdes.
...	Possible extra arguments for plotting dataframes

Examples

```
rri <- opt_des(Criterion = "I-Optimality", model = y ~ a * exp(-b / x),
  parameters = c("a", "b"), par_values = c(1, 1500), design_space = c(212, 422),
  reg_int = c(380, 422))
plot(rri)
```

---

plot_convergence   *Plot Convergence of the algorithm*

Description

Plots the criterion value on each of the steps of the algorithm, both for optimizing weights and points, against the total step number.

Usage

```
plot_convergence(convergence)
```

Arguments

convergence   A dataframe with two columns:

- `criteria` contains value of the criterion on each step.
- `step` contains number of the step.

Value

A ggplot object with the `criteria` in the y axis and `step` in the x axis.

---

plot_sens   *Plot sensitivity function*

Description

Plots the sensitivity function and the value of the Equivalence Theorem as an horizontal line, which helps assess the optimality of the design of the given sensitivity function.

Usage

```
plot_sens(min, max, sens_function, criterion_value)
```

Arguments

min   Minimum of the space of the design, used in the limits of the representation.

max   Maximum of the space of the design, used in the limits of the representation.

sens_function   A single variable function, the sensitivity function.

criterion_value

A numeric value representing the other side of the inequality of the Equivalence Theorem.

Value

A `ggplot` object that represents the sensitivity function

---

print.optdes   *Print function for optdes*

Description

Print function for optdes

Usage

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

Arguments

x   An object of class optdes.

...   Possible extra arguments for printing dataframes

Examples

```
rri <- opt_des(Criterion = "I-Optimality", model = y ~ a * exp(-b / x),
  parameters = c("a", "b"), par_values = c(1, 1500), design_space = c(212, 422),
  reg_int = c(380, 422))
print(rri)
```

---

sens   *Master function to calculate the sensitivity function*

Description

Calculates the sensitivity function given the desired Criterion, an information matrix and other necessary values depending on the chosen criterion.

Usage

```
sens(Criterion, grad, M, par_int = c(1), matB = NA)
```

Arguments

Criterion   character variable with the chosen optimality criterion. Can be one of the following:

      • 'D-Optimality'

      • 'Ds-Optimality'

      • 'A-Optimality'

      • 'I-Optimality'

grad	A function in a single variable that returns the partial derivatives vector of the model.
M	Information Matrix for the sensitivity function.
par_int	Numeric vector of the indexes of the parameters of interest for Ds-Optimality.
matB	Matrix resulting from the integration of the one-point Information Matrix along the interest region.

Value

The sensitivity function as a matrix of single variable.

---

shiny_augment	*Shiny D-augment*

Description

Launches the demo shiny application to D-augment several prespecified models

Usage

```
shiny_augment()
```

Examples

```
shiny_augment()
```

---

shiny_optimal	*Shiny Optimal*

Description

Launches the demo shiny application to calculate optimal designs for Antoine's Equation

Usage

```
shiny_optimal()
```

Examples

```
shiny_optimal()
```

---

summary.optdes   *Summary function for optdes*

Description

Summary function for optdes

Usage

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

Arguments

object   An object of class optdes.

...   Possible extra arguments for the summary

Examples

```
rri <- opt_des(Criterion = "I-Optimality", model = y ~ a * exp(-b / x),
  parameters = c("a", "b"), par_values = c(1, 1500), design_space = c(212, 422),
  reg_int = c(380, 422))
summary(rri)
```

---

tr   *Trace*

Description

Return the mathematical trace of a matrix, the sum of its diagonal elements.

Usage

```
tr(M)
```

Arguments

M   The matrix from which to calculate the trace.

Value

The trace of the matrix.

---

update_design   *Update Design with new point*

Description

Updates a design adding a new point to it. If the added point is closer than `delta` to an existing point of the design, the two points are merged together as their arithmetic average. Then updates the weights to be equal to all points of the design.

Usage

```
update_design(design, xmax, delta, new_weight)
```

Arguments

design   Design to update. It's a dataframe with two columns:
                - `Point` contains the support points of the design.
                - `Weight` contains the corresponding weights of the `Points`.
xmax   The point to add as a numeric value.
delta   Threshold which defines how close the new point has to be to any of the existing ones in order to merge with them.
new_weight   Number with the weight for the new point.

Value

The updated design.

---

update_design_total   *Merge close points of a design*

Description

Takes a design and merge together all points that are closer between them than a certain threshold `delta`.

Usage

```
update_design_total(design, delta)
```

Arguments

design   The design to update. It's a dataframe with two columns:
                - `Point` contains the support points of the design.
                - `Weight` contains the corresponding weights of the `Points`.
delta   Threshold which defines how close two points have to be to any of the existing ones in order to merge with them.

Value

The updated design.

---

update_sequence | *Deletes duplicates points*

Description

Within a vector of points, deletes points that are close enough (less than the tol parameter). Returns the points without the "duplicates"

Usage

```
update_sequence(points, tol)
```

Arguments

points   Points to be updated

tol   Tolerance for which two points are considered the same

Value

The points without duplicates

---

update_weights | *Update weight D-Optimality*

Description

Implementation of the weight update formula for D-Optimality used to optimize the weights of a design, which is to be applied iteratively until no sizable changes happen.

Usage

```
update_weights(design, sens, k, delta)
```

Arguments

design   Design to optimize the weights from. It's a dataframe with two columns:

- Point contains the support points of the design.
- Weight contains the corresponding weights of the Points.

sens   Sensibility function for the design and model.

k   Number of parameters of the model.

delta   A parameter of the algorithm that can be tuned. Must be $0 < delta < 1$.

Value

returns the new weights of the design after one iteration.

---

update_weightsDS   *Update weight Ds-Optimality*

Description

Implementation of the weight update formula for Ds-Optimality used to optimize the weights of a design, which is to be applied iteratively until no sizable changes happen.

Usage

```
update_weightsDS(design, sens, s, delta)
```

Arguments

design	Design to optimize the weights from. It's a dataframe with two columns:
	• Point contains the support points of the design.
	• Weight contains the corresponding weights of the Points.
sens	Sensibility function for the design and model.
s	number of parameters of interest of the model
delta	A parameter of the algorithm that can be tuned. Must be $0 < delta < 1$.

Value

returns the new weights of the design after one iteration.

---

update_weightsI   *Update weight I-Optimality*

Description

Implementation of the weight update formula for I-Optimality used to optimize the weights of a design, which is to be applied iteratively until no sizable changes happen. A-Optimality if instead of the integral matrix the identity function is used.

Usage

```
update_weightsI(design, sens, crit, delta)
```

Arguments

`design`	Design to optimize the weights from. It's a dataframe with two columns:

- `Point` contains the support points of the design.
- `Weight` contains the corresponding weights of the `Points`.

`sens`	Sensibility function for the design and model.
`crit`	Value of the criterion function for I-Optimality.
`delta`	A parameter of the algorithm that can be tuned. Must be $0 < delta < 1$.

Value

returns the new weights of the design after one iteration.

`weight_function`	*Weight function per distribution*

Description

Weight function per distribution

Usage

```
weight_function(model, char_vars, values, distribution = "Homoscedasticity")
```

Arguments

`model`	formula describing the model to use. Must use x as the variable.
`char_vars`	character vector with the parameters of the models, as written in the `formula`
`values`	numeric vector with the parameters nominal values, in the same order as given in `parameters`.
`distribution`	character variable specifying the probability distribution of the response. Can be one of the following:

- 'Homoscedasticity'
- 'Gamma', which can be used for exponential or normal heteroscedastic with constant relative error
- 'Poisson'
- 'Logistic'
- 'Log-Normal' (work in progress)

Value

one variable function that represents the square of the structure of variance, in case of heteroscedastic variance of the response.

WFMult | *Master function for the cocktail algorithm, that calls the appropriate one given the criterion.*

Description

Depending on the `Criterion` the cocktail algorithm for the chosen criterion is called, and the necessary parameters for the functions are given from the user input.

Usage

```
WFMult(
  init_design,
  grad,
  Criterion,
  par_int = NA,
  matB = NA,
  min,
  max,
  grid.length,
  join_thresh,
  delete_thresh,
  k,
  delta_weights,
  tol,
  tol2
)
```

Arguments

init_design
: optional dataframe with the initial design for the algorithm. A dataframe with two columns:

  - `Point` contains the support points of the design.
  - `Weight` contains the corresponding weights of the `Points`.

grad
: function of partial derivatives of the model.

Criterion
: character variable with the chosen optimality criterion. Can be one of the following:

  - 'D-Optimality'
  - 'Ds-Optimality'
  - 'A-Optimality'
  - 'I-Optimality'

par_int
: numeric vector with the index of the `parameters` of interest. Only necessary when the `Criterion` chosen is 'Ds-Optimality'.

matB
: optional matrix of dimensions k x k, integral of the information matrix of the model over the interest region for I-optimality.

min	numeric value with the inferior bound of the space of the design.
max	numeric value with the upper bound of the space of the design.
grid.length	numeric value that gives the grid to evaluate the sensitivity function when looking for a maximum.
join_thresh	numeric value that states how close, in real units, two points must be in order to be joined together by the join heuristic.
delete_thresh	numeric value with the minimum weight, over 1 total, that a point needs to have in order to not be deleted from the design.
k	number of unknown parameters of the model.
delta_weights	numeric value in (0, 1), parameter of the algorithm.
tol	numeric value for the convergence of the weight optimizing algorithm.
tol2	numeric value for the stop condition of the algorithm.

Value

list correspondent to the output of the correspondent algorithm called, dependent on the criterion. A list of two objects:

- optdes: a dataframe with the optimal design in two columns, `Point` and `Weight`.
- sens: a plot with the sensitivity function to check for optimality of the design.

See Also

Other cocktail algorithms: `DWFMult()`, `DsWFMult()`, `IWFMult()`

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