# Package: GreedyExperimentalDesign (via r-universe)

October 26, 2024

Type Package

Title Greedy Experimental Design Construction

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Description Computes experimental designs for a two-arm experiment with covariates via a number of methods: (0) complete randomization and randomization with forced-balance, (1) Greedily optimizing a balance objective function via pairwise switching. This optimization provides lower variance for the treatment effect estimator (and higher power) while preserving a design that is close to complete randomization. We return all iterations of the designs for use in a permutation test, (2) The second is via numerical optimization (via 'gurobi' which must be installed, see

<https://www.gurobi.com/documentation/9.1/quickstart\_windows/r\_ins\_the\_r\_
package.html>)

a la Bertsimas and Kallus, (3) rerandomization, (4) Karp's method for one covariate, (5) exhaustive enumeration to find the optimal solution (only for small sample sizes), (6) Binary pair matching using the 'nbpMatching' library, (7) Binary pair matching plus design number (1) to further optimize balance, (8) Binary pair matching plus design number (3) to further optimize balance, (9) Hadamard designs, (10) Simultaneous Multiple Kernels. In (1-9) we allow for three objective functions: Mahalanobis distance, Sum of absolute differences standardized and Kernel distances via the 'kernlab' library. This package is the result of a stream of research that can be found in Krieger, A, Azriel, D and Kapelner, A ``Nearly Random Designs with Greatly Improved Balance" (2016) <arXiv:1612.02315>, Krieger, A, Azriel, D and Kapelner, A ``Better Experimental Design by Hybridizing Binary Matching with Imbalance Optimization" (2021) <arXiv:2012.03330>.

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## Description

The automobile data frame has 201 rows and 25 columns and concerns automobiles in the 1985 Auto Imports Database. The response variable, price, is the log selling price of the automobile. There are 7 categorical predictors and 17 continuous / integer predictors which are features of the automobiles. 41 automobiles have missing data in one or more of the feature entries. This dataset is true to the original except with a few of the predictors dropped.

## Usage

data(automobile)

#### **Source**

K Bache and M Lichman. UCI machine learning repository, 2013. http://archive.ics.uci.edu/ml/datasets/Automobile

complete\_randomization

*Implements complete randomization (without forced balance)* 

## Description

For debugging, you can use set. seed to be assured of deterministic output.

## Usage

```
complete_randomization(n, r, form = "one_zero")
```

#### **Arguments**

n number of observations

r number of randomized designs you would like

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

#### Value

a matrix where each column is one of the r designs

#### Author(s)

Adam Kapelner

## **Description**

For debugging, you can use set. seed to be assured of deterministic output.

## Usage

```
complete_randomization_with_forced_balanced(n, r, form = "one_zero")
```

#### **Arguments**

n number of observations

r number of randomized designs you would like

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

#### Value

a matrix where each column is one of the r designs

## Author(s)

Adam Kapelner

computeBinaryMatchStructure

Compute Binary Matching Strcuture

#### **Description**

This method creates an object of type binary\_match\_structure and will compute pairs. You can then use the functions initBinaryMatchExperimentalDesignSearch and resultsBinaryMatchSearch to create randomized allocation vectors. For one column in X, we just sort to find the pairs trivially.

## Usage

```
computeBinaryMatchStructure(
   X,
   mahal_match = FALSE,
   compute_dist_matrix = NULL,
   D = NULL
)
```

## **Arguments**

Χ

The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one for each measurement on the subject). This is the design matrix you wish to search for a more optimal design.

mahal\_match

Match using Mahalanobis distance. Default is FALSE.

compute\_dist\_matrix

The function that computes the distance matrix between every two observations in X, its only argument. The default is NULL signifying euclidean squared distance optimized in C++.

D

A distance matrix precomputed. The default is NULL indicating the distance matrix should be computed.

## Value

An object of type binary\_experimental\_design which can be further operated upon.

## Author(s)

Adam Kapelner

compute\_gram\_matrix

Gram Matrix Computation

## Description

Computes the Gram Matrix for a user-specified kernel using the library kernlab. Note that this function automatically standardizes the columns of the data entered.

## Usage

```
compute_gram_matrix(X, kernel_type, params = c())
```

## **Arguments**

X The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one

for each measurement on the subject). This is the design matrix you wish to

search for a more optimal design.

kernel\_type One of the following: "vanilla", "rbf", "poly", "tanh", "bessel", "laplace", "anova"

or "spline".

params A vector of numeric parameters. Each kernel\_type has different numbers of

parameters required. For more information see documentation for the kernlab

library.

#### Value

The n x n gram matrix for the given kernel on the given data.

## Author(s)

compute\_objective\_val Computes Objective Value From Allocation Vector

## **Description**

Returns the objective value given a design vector as well an an objective function. This is sometimes duplicated in Java. However, within Java, tricks are played to make optimization go faster so Java's objective values may not always be the same as the true objective function (e.g. logs or constants dropped).

## Usage

```
compute_objective_val(X, indic_T, objective = "abs_sum_diff", inv_cov_X = NULL)
```

## Arguments

X The n x p design matrix

indic\_T The n-length binary allocation vector

objective The objective function to use. Default is abs\_sum\_diff and the other option is

mahal\_dist.

inv\_cov\_X Optional: the inverse sample variance covariance matrix. Use this argument if

you will be doing many calculations since passing this in will cache this data.

#### Author(s)

Adam Kapelner

compute\_randomization\_metrics

Computes Randomization Metrics (explained in paper) about a design algorithm

#### **Description**

Computes Randomization Metrics (explained in paper) about a design algorithm

## Usage

```
compute_randomization_metrics(designs)
```

## Arguments

designs A matrix where each column is one design.

#### Value

A list of resulting data: the probability estimates for each pair in the design of randomness where estmates close to ~0.5 represent random assignment, then the entropy metric the distance metric, the maximum eigenvalue of the allocation var-cov matrix (operator norm) and the squared Frobenius norm (the sum of the squared eigenvalues)

#### Author(s)

Adam Kapelner

```
generate_stdzied_design_matrix
```

Generates a design matrix with standardized predictors.

## **Description**

This function is useful for debugging.

## Usage

```
generate_stdzied_design_matrix(n = 50, p = 1, covariate_gen = rnorm, ...)
```

#### **Arguments**

n Number of rows in the design matrix

p Number of columns in the design matrix

covariate\_gen The function to use to draw the covariate realizations (assumed to be iid). This

defaults to rnorm for N(0,1) draws.

... Optional arguments to be passed to the covariate\_dist function.

## Value

THe design matrix

#### Author(s)

GreedyExperimentalDesign

Greedy Experimental Design Search

## **Description**

A tool to find many types of a priori experimental designs

## Author(s)

Adam Kapelner <kapelner@qc.cuny.edu>

#### References

Kapelner, A

greedy\_orthogonalization\_curation

Curate More Orthogonal Vectors Greedily

#### **Description**

This function takes a set of allocation vectors and pares them down one-by-one by eliminating the vector that can result in the largest reduction in Avg[ |r\_ij| ]. It is recommended to begin with a set of unmirrored vectors for speed. Then add the mirrors later for whichever subset you wish.

#### Usage

```
greedy_orthogonalization_curation(W, Rmin = 2, verbose = FALSE)
```

#### **Arguments**

W A matrix in \$-1, 1^R x n\$ which have R allocation vectors for an experiment of

sample size n.

Rmin The minimum number of vectors to consider in a design. The default is the true

bottom, two.

verbose Default is FALSE but if not, it will print out a message for each iteration.

#### Value

A list with two elements: (1)  $avg_abs_rij_by_R$  which is a data frame with R - Rmin + 1 rows and columns R and average absolute  $r_ij$  and (2) Wsorted which provides the collection of vectors in sorted by best average absolute  $r_ij$  in row order from best to worst.

#### Author(s)

greedy\_orthogonalization\_curation2

Curate More Orthogonal Vectors Greedily

## **Description**

This function takes a set of allocation vectors and pares them down one-by-one by eliminating the vector that can result in the largest reduction in Avg[ |r\_ij| ]. It is recommended to begin with a set of unmirrored vectors for speed. Then add the mirrors later for whichever subset you wish.

### Usage

```
greedy_orthogonalization_curation2(W, R0 = 100, verbose = FALSE)
```

#### **Arguments**

W A matrix in \$-1, 1^R x n\$ which have R allocation vectors for an experiment of

sample size n.

R0 The minimum number of vectors to consider in a design. The default is the true

bottom, two.

verbose Default is FALSE but if not, it will print out a message for each iteration.

#### Value

A list with two elements: (1)  $avg_abs_rij_by_R$  which is a data frame with R - Rmin + 1 rows and columns R and average absolute  $r_ij$  and (2) Wsorted which provides the collection of vectors in sorted by best average absolute  $r_ij$  in row order from best to worst.

## Author(s)

Adam Kapelner

hadamardExperimentalDesign

Create a Hadamard Design

## **Description**

This method returns unique designs according to a Hadamard matrix. For debugging, you can use set.seed to be assured of deterministic output.

#### Usage

```
hadamardExperimentalDesign(X, strict = TRUE, form = "zero_one")
```

#### **Arguments**

X The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one

for each measurement on the subject). The measurements aren't used to com-

pute the Hadamard designs, only the number of rows.

strict Hadamard matrices are not available for all \$n\$.

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

#### Value

An matrix of dimension \$R\$ x \$n\$ where \$R\$ is the number of Hadamard allocations.

#### Author(s)

Adam Kapelner

imbalanced\_block\_designs

Implements unequally allocated block designs

#### **Description**

For debugging, you can use set.seed to be assured of deterministic output. The following quantities in this design must be integer valued or an error will be thrown:  $n_B := n / B$  and  $n_B * prop_T$ 

### Usage

```
imbalanced_block_designs(n, prop_T, B, r, form = "one_zero")
```

#### **Arguments**

n number of observations

prop\_T the proportion of treatments needed

B the number of blocks

r number of randomized designs you would like

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

#### Value

a matrix where each column is one of the r designs

## Author(s)

imbalanced\_complete\_randomization

Implements unequally allocated complete randomization

## **Description**

For debugging, you can use set. seed to be assured of deterministic output.

#### Usage

```
imbalanced_complete_randomization(n, prop_T, r, form = "one_zero")
```

## Arguments

n number of observations

prop\_T the proportion of treatments needed

r number of randomized designs you would like

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

#### Value

a matrix where each column is one of the r designs

## Author(s)

Adam Kapelner

 ${\it initBinaryMatchExperimentalDesignSearch} \\ {\it Begin~a~Binary~Match~Search}$ 

## **Description**

This method creates an object of type pairwise\_matching\_experimental\_design\_search and will immediately initiate a search through \$1\_T\$ space for pairwise match designs based on the structure computed in the function computeBinaryMatchStructure. For debugging, you can use set the seed parameter and num\_cores = 1 to be assured of deterministic output.

#### Usage

```
initBinaryMatchExperimentalDesignSearch(
  binary_match_structure,
  max_designs = 1000,
  wait = FALSE,
  start = TRUE,
  num_cores = 1,
  seed = NULL,
  prop_flips = 1
)
```

#### **Arguments**

binary\_match\_structure

The binary\_experimental\_design object where the pairs are computed.

max\_designs How many random allocation vectors you wish to return. The default is 1000.

wait Should the R terminal hang until all max\_designs vectors are found? The default

is FALSE.

start Should we start searching immediately (default is TRUE).

num\_cores The number of CPU cores you wish to use during the search. The default is 1.

seed The set to set for deterministic output. This should only be set if num\_cores = 1

otherwise the output will not be deterministic. Default is NULL for no seed set.

prop\_flips Proportion of flips. Default is all. Lower for more correlated assignments (useful

for research only).

#### Author(s)

Adam Kapelner

 $in it Binary {\tt MatchFollowedByGreedyExperimentalDesignSearch}$ 

Begin a Search for Binary Matching Followed by Greedy Switch Designs

## Description

This method creates an object of type binary\_then\_greedy\_experimental\_design and will find optimal matched pairs which are then greedily switched in order to further minimize a balance metric. You can then use the function resultsBinaryMatchThenGreedySearch to obtain the randomized allocation vectors. For one column in X, the matching just sorts the values to find the pairs trivially.

#### Usage

```
initBinaryMatchFollowedByGreedyExperimentalDesignSearch(
   X,
   diff_method = FALSE,
   compute_dist_matrix = NULL,
   ...
)
```

#### **Arguments**

Χ

The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one for each measurement on the subject). This is the design matrix you wish to search for a more optimal design.

diff\_method

Once the subjects (i.e. row vectors) are paired, do we create a set of \$n\$/2 difference vectors and feed that into greedy? If TRUE, this technically breaks the objective function, but it is shown to have better performance. The default is thus FALSE.

compute\_dist\_matrix

The function that computes the distance matrix between every two observations in X, its only argument. The default is NULL signifying euclidean squared distance optimized in C++.

. . .

Arguments passed to initGreedyExperimentalDesignObject. It is recommended to set max\_designs otherwise it will default to 10,000.

#### Value

An object of type binary\_experimental\_design which can be further operated upon.

#### Author(s)

Adam Kapelner

 $in it Binary {\tt MatchFollowedByRerandomizationDesignSearch}$ 

Begin a Search for Binary Matching Followed by Rerandomization

#### **Description**

This method creates an object of type binary\_then\_rerandomization\_experimental\_design and will find optimal matched pairs which are then rerandomized in order to further minimize a balance metric. You can then use the function resultsBinaryMatchThenRerandomizationSearch to obtain the randomized allocation vectors. For one column in X, the matching just sorts the values to find the pairs trivially.

#### Usage

```
initBinaryMatchFollowedByRerandomizationDesignSearch(
   X,
   compute_dist_matrix = NULL,
   ...
)
```

#### **Arguments**

Χ

The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one for each measurement on the subject). This is the design matrix you wish to search for a more optimal design.

compute\_dist\_matrix

The function that computes the distance matrix between every two observations in X, its only argument. The default is NULL signifying euclidean squared distance optimized in C++.

Arguments passed to initGreedyExperimentalDesignObject. It is recommended to set max\_designs otherwise it will default to 10,000.

#### Value

An object of type binary\_experimental\_design which can be further operated upon.

#### Author(s)

Adam Kapelner

init Greedy Experimental Design Object

Begin A Greedy Pair Switching Search

## **Description**

This method creates an object of type greedy\_experimental\_design and will immediately initiate a search through \$1\_T\$ space for forced balance designs. For debugging, you can use set the seed parameter and num\_cores = 1 to be assured of deterministic output.

## Usage

```
initGreedyExperimentalDesignObject(
  X = NULL,
  nT = NULL,
  max_designs = 10000,
  objective = "mahal_dist",
  indicies_pairs = NULL,
  Kgram = NULL,
```

```
wait = FALSE,
start = TRUE,
max_iters = Inf,
semigreedy = FALSE,
diagnostics = FALSE,
num_cores = 1,
seed = NULL
)
```

#### **Arguments**

X The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one for each measurement on the subject). This is the design matrix you wish to search for a more optimal design. This parameter must be specified unless you

choose objective type "kernel" in which case, the Kgram parameter must be

specified.

nT The number of treatments to assign. Default is NULL which is for forced balance

allocation i.e. nT = nC = n/2 where n is the number of rows in X (or Kgram if

X is unspecified).

max\_designs The maximum number of designs to be returned. Default is 10,000. Make this

large so you can search however long you wish as the search can be stopped at

any time by using the stopSearch method

objective The objective function to use when searching design space. This is a string with

valid values "mahal\_dist" (the default), "abs\_sum\_diff" or "kernel".

indicies\_pairs A matrix of size \$n/2\$ times 2 whose rows are indicies pairs. The values of the

entire matrix must enumerate all indicies \$1, ..., n\$. The default is NULL meaning

to use all possible pairs.

Kgram If the objective = kernel, this argument is required to be an  $n \times n$  matrix

whose entries are the evaluation of the kernel function between subject i and

subject j. Default is NULL.

wait Should the R terminal hang until all max\_designs vectors are found? The deafult

is FALSE.

start Should we start searching immediately (default is TRUE).

max\_iters Should we impose a maximum number of greedy switches? The default is Inf

which a flag for "no limit."

semigreedy Should we use a fully greedy approach or the quicker semi-greedy approach?

The default is FALSE corresponding to the fully greedy approach.

diagnostics Returns diagnostic information about the iterations including (a) the initial start-

ing vectors, (b) the switches at every iteration and (c) information about the objective function at every iteration (default is FALSE to decrease the algorithm's

run time).

num\_cores The number of CPU cores you wish to use during the search. The default is 1.

seed The set to set for deterministic output. This should only be set if num\_cores = 1

otherwise the output will not be deterministic. Default is NULL for no seed set.

#### Value

An object of type greedy\_experimental\_design\_search which can be further operated upon

#### Author(s)

Adam Kapelner

#### **Examples**

```
## Not run:
library(MASS)
data(Boston)
#pretend the Boston data was an experiment setting
#first pull out the covariates
X = Boston[, 1 : 13]
#begin the greedy design search
ged = initGreedyExperimentalDesignObject(X,
    max_designs = 1000, num_cores = 3, objective = "abs_sum_diff")
#wait
ged
## End(Not run)
```

init Greedy Multiple Kernel Experimental Design Object

Begin A Greedy Pair Multiple Kernel Switching Search

#### **Description**

This method creates an object of type greedy\_multiple\_kernel\_experimental\_design and will immediately initiate a search through \$1\_T\$ space for forced balance designs. For debugging, you can use set the seed parameter and num\_cores = 1 to be assured of deterministic output.

## Usage

```
initGreedyMultipleKernelExperimentalDesignObject(
   X = NULL,
   max_designs = 10000,
   objective = "added_pct_reduction",
   kernel_pre_num_designs = 2000,
   kernel_names = NULL,
   Kgrams = NULL,
   maximum_gain_scaling = 1.1,
   kernel_weights = NULL,
   wait = FALSE,
   start = TRUE,
   max_iters = Inf,
   semigreedy = FALSE,
```

```
diagnostics = FALSE,
 num\_cores = 1,
  seed = NULL
)
```

#### **Arguments**

Χ

The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one for each measurement on the subject). This is the design matrix you wish to search for a more optimal design. We will standardize this matrix by column internally.

max\_designs

The maximum number of designs to be returned. Default is 10,000. Make this large so you can search however long you wish as the search can be stopped at any time by using the stopSearch method

objective

The method used to aggregate the kernel objective functions together. Default is "added\_pct\_reduction".

kernel\_pre\_num\_designs

How many designs per kernel to run to explore the space of kernel objective values. Default is 2000.

kernel\_names

An array with the kernels to compute with default parameters. Must have elements in the following set: "mahalanobis", "poly\_s" where the "s" is a natural number 1 or greater, "exponential", "laplacian", "inv\_mult\_quad", "gaussian". Default is NULL to indicate the kernels are specified manually using the Kgrams parameter.

Kgrams

A list of M >= 1 elements where each is a n x n matrix whose entries are the evaluation of the kernel function between subject i and subject j. Default is NULL to indicate this was specified using the convenience parameter kernel\_names.

maximum\_gain\_scaling

This controls how much the percentage of possible improvement on a kernel objective function should be scaled by. The minimum is 1 which allows for designs that could potentially have >=100 improvement over original. We recommend 1.1 which means that a design that was found to be the best of the kernel\_pre\_num\_designs still has 1/1.1 = 9% room to grow making it highly unlikely that any design could be  $\geq 100\%$ .

kernel\_weights

A vector with positive weights (need not be normalized) where each element represents the weight of each kernel. The default is NULL for uniform weighting.

wait

Should the R terminal hang until all max\_designs vectors are found? The deafult is FALSE.

start

Should we start searching immediately (default is TRUE).

max\_iters

Should we impose a maximum number of greedy switches? The default is Inf which a flag for "no limit."

semigreedy

Should we use a fully greedy approach or the quicker semi-greedy approach? The default is FALSE corresponding to the fully greedy approach.

diagnostics

Returns diagnostic information about the iterations including (a) the initial starting vectors, (b) the switches at every iteration and (c) information about the objective function at every iteration (default is FALSE to decrease the algorithm's run time).

num\_cores The number of CPU cores you wish to use during the search. The default is 1.

The set to set for deterministic output. This should only be set if num\_cores = 1 otherwise the output will not be deterministic. Default is NULL for no seed set.

Value

An object of type greedy\_experimental\_design\_search which can be further operated upon

#### Author(s)

Adam Kapelner

#### **Examples**

```
## Not run:
library(MASS)
data(Boston)
#pretend the Boston data was an experiment setting
#first pull out the covariates
X = Boston[, 1 : 13]
#begin the greedy design search
ged = initGreedyMultipleKernelExperimentalDesignObject(X,
    max_designs = 1000, num_cores = 3, kernel_names = c("mahalanobis", "gaussian"))
#wait
ged
## End(Not run)
```

initKarpExperimentalDesignObject

Begin Karp Search

## **Description**

This method creates an object of type karp\_experimental\_design and will immediately initiate a search through \$1\_T\$ space. Note that the Karp search only works for one covariate (i.e. \$p=1\$) and the objective "abs\_sum\_diff".

#### Usage

```
initKarpExperimentalDesignObject(
   X,
   wait = FALSE,
   balanced = TRUE,
   start = TRUE
)
```

#### **Arguments**

wait

Χ	The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one
	for each measurement on the subject). This is the design matrix you wish to
	search for a more karn design

search for a more karp design.

Should the R terminal hang until all max\_designs vectors are found? The deafult

is FALSE.

balanced Should the final vector be balanced? Default and recommended is TRUE.

start Should we start searching immediately (default is TRUE).

#### Value

An object of type karp\_experimental\_design\_search which can be further operated upon

#### Author(s)

Adam Kapelner

initOptimalExperimentalDesignObject

Begin a Search for the Optimal Solution

#### **Description**

This method creates an object of type optimal\_experimental\_design and will immediately initiate a search through \$1\_T\$ space. Since this search takes exponential time, for most machines, this method is futile beyond 28 samples. You've been warned! For debugging, you can use set num\_cores = 1 to be assured of deterministic output.

#### Usage

```
initOptimalExperimentalDesignObject(
  X = NULL,
  objective = "mahal_dist",
  Kgram = NULL,
  wait = FALSE,
  start = TRUE,
  num_cores = 1
)
```

#### **Arguments**

X The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one

for each measurement on the subject). This is the design matrix you wish to

search for a more optimal design.

objective The objective function to use when searching design space. This is a string with

valid values "mahal\_dist" (the default), "abs\_sum\_diff" or "kernel".

Kgram	If the objective = kernel, this argument is required to be an n x n matrix whose entries are the evaluation of the kernel function between subject i and subject j. Default is NULL.
wait	Should the R terminal hang until all max_designs vectors are found? The deafult is FALSE.
start	Should we start searching immediately (default is TRUE).
num_cores	The number of CPU cores you wish to use during the search. The default is 1.

#### Value

An object of type optimal\_experimental\_design\_search which can be further operated upon

## Author(s)

Adam Kapelner

## Description

This method creates an object of type rerandomization\_experimental\_design and will immediately initiate a search through \$1\_T\$ space for forced-balance designs. For debugging, you can use set the seed parameter and num\_cores = 1 to be assured of deterministic output.

## Usage

```
initRerandomizationExperimentalDesignObject(
   X = NULL,
   obj_val_cutoff_to_include,
   max_designs = 1000,
   objective = "mahal_dist",
   Kgram = NULL,
   wait = FALSE,
   start = TRUE,
   num_cores = 1,
   seed = NULL
)
```

#### **Arguments**

Χ

The design matrix with \$n\$ rows (one for each subject) and \$p\$ columns (one for each measurement on the subject). This is the design matrix you wish to search for a more optimal design.

obj\_val\_cutoff\_to\_include

Only allocation vectors with objective values lower than this threshold will be returned. If the cutoff is infinity, you are doing BCRD and you should use the complete\_randomization\_with\_forced\_balanced function instead.

max\_designs The maximum number of designs to be returned. Default is 10,000. Make this

large so you can search however long you wish as the search can be stopped at

any time by using the stopSearch method

objective The objective function to use when searching design space. This is a string with

valid values "mahal\_dist" (the default), "abs\_sum\_diff" or "kernel".

Kgram If the objective = kernel, this argument is required to be an  $n \times n$  matrix

whose entries are the evaluation of the kernel function between subject i and

subject j. Default is NULL.

wait Should the R terminal hang until all max\_designs vectors are found? The default

is FALSE.

start Should we start searching immediately (default is TRUE).

num\_cores The number of CPU cores you wish to use during the search. The default is 1.

seed The set to set for deterministic output. This should only be set if num\_cores = 1

otherwise the output will not be deterministic. Default is NULL for no seed set.

#### Value

An object of type rerandomization\_experimental\_design\_search which can be further operated upon.

#### Author(s)

Adam Kapelner

```
optimize_asymmetric_treatment_assignment
```

Compute Optimal Number of Treatments/Controls

#### **Description**

Given a total budget and asymmetric treatment and control costs, calculate the number of treatments and controls that optimize the variance of the estimator. The number of treatments is rounded up by default.

### Usage

```
optimize_asymmetric_treatment_assignment(
   c_treatment = NULL,
   c_control = NULL,
   c_total_max = NULL,
   n = NULL
)
```

#### **Arguments**

c_treatment	The cost of a treatment assignment. Default is NULL for symmetric costs.
c_control	The cost of a control assignment. Default is NULL for symmetric costs.
c_total_max	The total cost constraint of any allocation. Either this or n must be specified. Default is NULL.
n	The total cost constraint as specified by the total number of subjects. Either this or c_total must be specified. Default is NULL.

#### Value

A list with three keys: n, nT, nC plus specified arguments

## Author(s)

Adam Kapelner

## **Examples**

```
## Not run:
optimize_asymmetric_treatment_assignment(n = 100)
#nT = nC = 50
optimize_asymmetric_treatment_assignment(n = 100, c_treatment = 2, c_control = 1)
#nT = 66, nC = 34
optimize_asymmetric_treatment_assignment(c_total_max = 50, c_treatment = 2, c_control = 1)
## End(Not run)
```

```
plot.greedy_experimental_design_search
```

Plots a summary of a greedy search object object

## **Description**

Plots a summary of a greedy search object object

#### Usage

```
## S3 method for class 'greedy_experimental_design_search' plot(x, \ldots)
```

## **Arguments**

x The greedy search object object to be summarized in the plot

... Other parameters to pass to the default plot function

## Value

An array of order statistics from plot\_obj\_val\_order\_statistic as a list element

24 plot\_obj\_val\_by\_iter

#### Author(s)

Adam Kapelner

```
plot. \verb|greedy_multiple_kernel_experimental_design| \\ Plots \ a \ summary \ of \ a \ \texttt{greedy_multiple_kernel_experimental_design} \\ object
```

#### **Description**

Plots a summary of a greedy\_multiple\_kernel\_experimental\_design object

## Usage

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

### **Arguments**

x The greedy\_multiple\_kernel\_experimental\_design object to be summarized in the plot

... Other parameters to pass to the default plot function

#### Value

An array of order statistics from plot\_obj\_val\_order\_statistic as a list element

## Author(s)

Adam Kapelner

```
plot_obj_val_by_iter Plots the objective value by iteration
```

## **Description**

Plots the objective value by iteration

## Usage

```
plot_obj_val_by_iter(res, runs = NULL)
```

#### **Arguments**

res Results from a greedy search object

runs A vector of run indices you would like to see plotted (default is to plot the first

up to 9)

#### Author(s)

Adam Kapelner

```
plot_obj_val_order_statistic
```

Plots an order statistic of the object value as a function of number of searches

## Description

Plots an order statistic of the object value as a function of number of searches

#### Usage

```
plot_obj_val_order_statistic(
  obj,
  order_stat = 1,
  skip_every = 5,
  type = "o",
  ...
)
```

## Arguments

obj The greedy search object object whose search history is to be visualized order\_stat The order statistic that you wish to plot. The default is 1 for the minimum. skip\_every Plot every nth point. This makes the plot generate much more quickly. The

default is 5.

type The type parameter for plot.

... Other arguments to be passed to the plot function.

#### Value

An array of order statistics as a list element

#### Author(s)

```
print.binary_match_structure
```

Prints a summary of a binary\_match\_structure object

## **Description**

Prints a summary of a binary\_match\_structure object

#### Usage

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

#### **Arguments**

x The binary\_match\_structure object to be summarized in the console

... Other parameters to pass to the default print function

#### Author(s)

Adam Kapelner

```
print.binary\_then\_greedy\_experimental\_design \\ Prints~a~summary~of~a~binary\_then\_greedy\_experimental\_design\\ object
```

## **Description**

Prints a summary of a binary\_then\_greedy\_experimental\_design object

#### Usage

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

#### **Arguments**

x The binary\_then\_greedy\_experimental\_design object to be summarized in the console

... Other parameters to pass to the default print function

#### Author(s)

print.binary\_then\_rerandomization\_experimental\_design

 $\label{lem:prints} \textit{Prints a summary of a} \ \texttt{binary\_then\_rerandomization\_experimental\_design} \\ \textit{object}$ 

#### **Description**

Prints a summary of a binary\_then\_rerandomization\_experimental\_design object

#### Usage

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

Other parameters to pass to the default print function

## **Arguments**

x The binary\_then\_rerandomization\_experimental\_design object to be sum-

marized in the console

## Author(s)

Adam Kapelner

```
print.greedy_experimental_design_search
```

 $Prints\ a\ summary\ of\ a\ {\it greedy\_experimental\_design\_search}\ object$ 

## Description

Prints a summary of a greedy\_experimental\_design\_search object

## Usage

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

#### **Arguments**

x The greedy\_experimental\_design\_search object to be summarized in the console

... Other parameters to pass to the default print function

#### Author(s)

print.greedy\_multiple\_kernel\_experimental\_design

 $\label{lem:prints} \textit{Prints a summary of a} \ \texttt{greedy\_multiple\_kernel\_experimental\_design} \\ \textit{object}$ 

## **Description**

Prints a summary of a greedy\_multiple\_kernel\_experimental\_design object

## Usage

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

## Arguments

x The greedy\_multiple\_kernel\_experimental\_design object to be summa-

rized in the console

... Other parameters to pass to the default print function

## Author(s)

Adam Kapelner

print.karp\_experimental\_design\_search

Prints a summary of a karp\_experimental\_design\_search object

## **Description**

Prints a summary of a karp\_experimental\_design\_search object

#### Usage

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

## **Arguments**

x The karp\_experimental\_design\_search object to be summarized in the con-

... Other parameters to pass to the default print function

## Author(s)

```
\verb|print.optimal_experimental_design_search|\\
```

 $Prints \ a \ summary \ of \ a \ {\it optimal\_experimental\_design\_search} \ object$ 

#### **Description**

Prints a summary of a optimal\_experimental\_design\_search object

#### Usage

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

## Arguments

x The optimal\_experimental\_design\_search object to be summarized in the

console

... Other parameters to pass to the default print function

#### Author(s)

Adam Kapelner

```
print.pairwise_matching_experimental_design_search
```

 $\label{lem:prints} \textit{Prints a summary of a} \ \texttt{pairwise\_matching\_experimental\_design\_search} \\ \textit{object}$ 

## **Description**

Prints a summary of a pairwise\_matching\_experimental\_design\_search object

## Usage

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

## **Arguments**

x The pairwise\_matching\_experimental\_design\_search object to be summarized in the console

Other parameters to pass to the default print function

#### Author(s)

print.rerandomization\_experimental\_design\_search

 $\label{lem:prints} \textit{Prints a summary of a} \ \texttt{rerandomization\_experimental\_design\_search} \\ \textit{object}$ 

## **Description**

Prints a summary of a rerandomization\_experimental\_design\_search object

## Usage

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

## Arguments

x The rerandomization\_experimental\_design\_search object to be summa-

rized in the console

... Other parameters to pass to the default print function

#### Author(s)

Adam Kapelner

resultsBinaryMatchSearch

Binary Pair Match Search

## **Description**

Returns the results (thus far) of the binary pair match design search

#### Usage

```
resultsBinaryMatchSearch(obj, form = "one_zero")
```

### Arguments

obj The pairwise\_matching\_experimental\_design\_search object that is cur-

rently running the search

form Which form should the assignments be in? The default is one\_zero for 1/0's or

 $pos_one_min_one for +1/-1$ 's.

## Author(s)

 $results {\tt BinaryMatchThenGreedySearch}$ 

Returns unique allocation vectors that are binary matched

## **Description**

Returns unique allocation vectors that are binary matched

## Usage

```
resultsBinaryMatchThenGreedySearch(
  obj,
  num_vectors = NULL,
  compute_obj_vals = FALSE,
  form = "zero_one"
)
```

#### **Arguments**

obj The binary\_then\_greedy\_experimental\_design object where the pairs are

computed.

num\_vectors How many random allocation vectors you wish to return. The default is NULL

indicating you want all of them.

compute\_obj\_vals

Should we compute all the objective values for each allocation? Default is

FALSE.

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

### Author(s)

Adam Kapelner

 $results {\tt BinaryMatchThenRer} and {\tt omizationSearch}$ 

Returns unique allocation vectors that are binary matched

#### Description

Returns unique allocation vectors that are binary matched

32 resultsGreedySearch

#### Usage

```
resultsBinaryMatchThenRerandomizationSearch(
  obj,
  num_vectors = NULL,
  compute_obj_vals = FALSE,
  form = "zero_one"
)
```

## **Arguments**

obj The binary\_then\_greedy\_experimental\_design object where the pairs are

computed.

num\_vectors How many random allocation vectors you wish to return. The default is NULL

indicating you want all of them.

compute\_obj\_vals

Should we compute all the objective values for each allocation? Default is

FALSE.

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

#### Author(s)

Adam Kapelner

resultsGreedySearch

Returns the results (thus far) of the greedy design search

#### **Description**

Returns the results (thus far) of the greedy design search

#### Usage

```
resultsGreedySearch(obj, max_vectors = 9, form = "one_zero")
```

#### **Arguments**

obj The greedy\_experimental\_design object that is currently running the search

This is not recommended as returning over 1,000 vectors is time-intensive. The

default is 9.

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

#### Author(s)

resultsKarpSearch 33

## **Examples**

```
## Not run:
library(MASS)
data(Boston)
#pretend the Boston data was an experiment setting
#first pull out the covariates
X = Boston[, 1 : 13]
#begin the greedy design search
ged = initGreedyExperimentalDesignObject(X,
 max_designs = 1000, num_cores = 2, objective = "abs_sum_diff")
#wait
res = resultsGreedySearch(ged, max_vectors = 2)
design = res$ending_indicTs[, 1] #ordered already by best-->worst
design
#what is the balance on this vector?
res$obj_vals[1]
#compute balance explicitly in R to double check
compute_objective_val(X, design) #same as above
#how far have we come?
ged
#we can cut it here
stopSearch(ged)
## End(Not run)
```

resultsKarpSearch

Returns the results (thus far) of the karp design search

## Description

Returns the results (thus far) of the karp design search

#### Usage

```
resultsKarpSearch(obj)
```

## **Arguments**

obj

The karp\_experimental\_design object that is currently running the search

## Author(s)

resultsMultipleKernelGreedySearch

Returns the results (thus far) of the greedy design search for multiple kernels

## Description

Returns the results (thus far) of the greedy design search for multiple kernels

#### Usage

```
resultsMultipleKernelGreedySearch(obj, max_vectors = 9, form = "one_zero")
```

### **Arguments**

obj The greedy\_multiple\_kernel\_experimental\_design object that is currently

running the search

max\_vectors The number of design vectors you wish to return. NULL returns all of them.

This is not recommended as returning over 1,000 vectors is time-intensive. The

default is 9.

form Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one

for +1/-1's.

#### Author(s)

Adam Kapelner

#### **Examples**

```
## Not run:
library(MASS)
data(Boston)
#pretend the Boston data was an experiment setting
#first pull out the covariates
X = Boston[, 1 : 13]
#begin the greedy design search
ged = initGreedyMultipleKernelExperimentalDesignObject(X,
 max_designs = 1000, num_cores = 3, kernel_names = c("mahalanobis", "gaussian"))
#wait
res = resultsMultipleKernelGreedySearch(ged, max_vectors = 2)
design = res$ending_indicTs[, 1] #ordered already by best-->worst
#how far have we come of the 1000 we set out to do?
#we can cut it here
stopSearch(ged)
## End(Not run)
```

resultsOptimalSearch 35

resultsOptimalSearch Returns the results (thus far) of the optimal design search

**Description** 

Returns the results (thus far) of the optimal design search

#### Usage

```
resultsOptimalSearch(obj, num_vectors = 2, form = "one_zero")
```

#### **Arguments**

obj The optimal\_experimental\_design object that is currently running the search num\_vectors

How many allocation vectors you wish to return. The default is 1 meaning the

best vector. If Inf, it means all vectors.

Which form should it be in? The default is one\_zero for 1/0's or pos\_one\_min\_one form

for +1/-1's.

#### Author(s)

Adam Kapelner

resultsRerandomizationSearch

Returns the results (thus far) of the rerandomization design search

## **Description**

Returns the results (thus far) of the rerandomization design search

#### Usage

```
resultsRerandomizationSearch(
  include_assignments = FALSE,
  form = "one_zero"
)
```

#### **Arguments**

The rerandomization\_experimental\_design object that is currently running obj

the search

include\_assignments

Do we include the assignments (takes time) and default is FALSE.

Which form should the assignments be in? The default is one\_zero for 1/0's or form

 $pos_one_min_one for +1/-1$ 's.

#### Author(s)

Adam Kapelner

searchTimeElapsed

Returns the amount of time elapsed

## **Description**

Returns the amount of time elapsed

## Usage

```
searchTimeElapsed(obj)
```

## **Arguments**

obj

The experimental\_design object that is currently running the search

## Author(s)

Adam Kapelner

standardize\_data\_matrix

Standardizes the columns of a data matrix.

## Description

Standardizes the columns of a data matrix.

## Usage

```
standardize_data_matrix(X)
```

## Arguments

Χ

The n x p design matrix

## Value

The n x p design matrix with columns standardized

## Author(s)

startSearch 37

startSearch

Starts the parallelized greedy design search.

## Description

Once begun, this function cannot be run again.

## Usage

```
startSearch(obj)
```

## **Arguments**

obj

The experimental\_design object that will be running the search

## Author(s)

Adam Kapelner

stopSearch

Stops the parallelized greedy design search.

## Description

Once stopped, it cannot be restarted.

## Usage

```
stopSearch(obj)
```

## Arguments

obj

The  $experimental\_design$  object that is currently running the search

## Author(s)

```
summary.binary_match_structure
```

Prints a summary of a binary\_match\_structure object

## **Description**

Prints a summary of a binary\_match\_structure object

#### Usage

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

#### **Arguments**

object The binary\_match\_structure object to be summarized in the console

Other parameters to pass to the default summary function

#### Author(s)

Adam Kapelner

```
summary.binary\_then\_greedy\_experimental\_design \\ Prints~a~summary~of~a~binary\_then\_greedy\_experimental\_design~object
```

## **Description**

Prints a summary of a binary\_then\_greedy\_experimental\_design object

#### Usage

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

#### **Arguments**

object The binary\_then\_greedy\_experimental\_design object to be summarized in

the console

... Other parameters to pass to the default summary function

#### Author(s)

summary.binary\_then\_rerandomization\_experimental\_design

Prints a summary of a binary\_then\_rerandomization\_experimental\_design
object

#### **Description**

Prints a summary of a binary\_then\_rerandomization\_experimental\_design object

#### Usage

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

## Arguments

object The binary\_then\_rerandomization\_experimental\_design object to be sum-

marized in the console

Other parameters to pass to the default summary function

#### Author(s)

Adam Kapelner

```
summary.greedy_experimental_design_search
```

 $Prints\ a\ summary\ of\ a\ {\it greedy\_experimental\_design\_search}\ object$ 

## **Description**

Prints a summary of a greedy\_experimental\_design\_search object

## Usage

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

## **Arguments**

object The greedy\_experimental\_design\_search object to be summarized in the

console

... Other parameters to pass to the default summary function

#### Author(s)

summary.greedy\_multiple\_kernel\_experimental\_design

 $\label{lem:prints} \textit{Prints a summary of a} \ \texttt{greedy\_multiple\_kernel\_experimental\_design} \\ \textit{object}$ 

## **Description**

Prints a summary of a greedy\_multiple\_kernel\_experimental\_design object

## Usage

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

## Arguments

object The greedy\_multiple\_kernel\_experimental\_design object to be summa-

rized in the console

... Other parameters to pass to the default summary function

## Author(s)

Adam Kapelner

summary.karp\_experimental\_design\_search

Prints a summary of a karp\_experimental\_design\_search object

## **Description**

Prints a summary of a karp\_experimental\_design\_search object

#### Usage

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

## **Arguments**

object The karp\_experimental\_design\_search object to be summarized in the con-

sole

... Other parameters to pass to the default summary function

## Author(s)

```
summary.optimal_experimental_design_search
```

 $Prints\ a\ summary\ of\ a\ {\it optimal\_experimental\_design\_search}\ object$ 

#### **Description**

Prints a summary of a optimal\_experimental\_design\_search object

#### Usage

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

## Arguments

object The optimal\_experimental\_design\_search object to be summarized in the

console

... Other parameters to pass to the default summary function

#### Author(s)

Adam Kapelner

```
summary.pairwise_matching_experimental_design_search
```

 $\label{lem:prints} \textit{Prints a summary of a} \ \texttt{pairwise\_matching\_experimental\_design\_search} \\ \textit{object}$ 

## **Description**

Prints a summary of a pairwise\_matching\_experimental\_design\_search object

## Usage

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

## Arguments

object The pairwise\_matching\_experimental\_design\_search object to be sum-

marized in the console

... Other parameters to pass to the default summary function

#### Author(s)

 $\verb|summary.rer| and \verb|omization_experimental_design_search| \\$ 

 $\label{lem:prints} \textit{Prints a summary of a} \ \texttt{rerandomization\_experimental\_design\_search} \\ \textit{object}$ 

## Description

Prints a summary of a rerandomization\_experimental\_design\_search object

## Usage

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

## Arguments

object The rerandomization\_experimental\_design\_search object to be summa-

rized in the console

... Other parameters to pass to the default summary function

#### Author(s)

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