

Package ‘GreedyExperimentalDesign’

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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](https://arxiv.org/abs/1612.02315)>,
Krieger, A, Azriel, D and Kapelner, A ``Better Experimental Design by Hybridizing Binary Matching with Imbalance Optimization" (2021) <[arXiv:2012.03330](https://arxiv.org/abs/2012.03330)>.

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Encoding UTF-8

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SystemRequirements Java (>= 7.0)

LinkingTo Rcpp

Imports Rcpp, checkmate, nbpMatching, survey, rlist, stringr, stringi, kernlab, graphics, grDevices, stats

URL <https://github.com/kapelner/GreedyExperimentalDesign>

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automobile

Data concerning automobile prices.

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 <code>one_zero</code> for 1/0's or <code>pos_one_min_one</code> for +1/-1's.

Value

a matrix where each column is one of the `r` designs

Author(s)

Adam Kapelner

```
complete_randomization_with_forced_balanced
    Implements forced balanced randomization
```

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

<code>n</code>	number of observations
<code>r</code>	number of randomized designs you would like
<code>form</code>	Which form should it be in? The default is <code>one_zero</code> for 1/0's or <code>pos_one_min_one</code> for +1/-1's.

Value

a matrix where each column is one of the `r` designs

Author(s)

Adam Kapelner

```
computeBinaryMatchStructure
    Compute Binary Matching Structure
```

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

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.
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 <code>kernel_type</code> has different numbers of parameters required. For more information see documentation for the <code>kernlab</code> library.

Value

The $n \times n$ gram matrix for the given kernel on the given data.

Author(s)

Adam Kapelner

`compute_objective_val` *Computes Objective Value From Allocation Vector*

Description

Returns the objective value given a design vector as well as 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

<code>X</code>	The $n \times p$ design matrix
<code>indic_T</code>	The n -length binary allocation vector
<code>objective</code>	The objective function to use. Default is <code>abs_sum_diff</code> and the other option is <code>mahal_dist</code> .
<code>inv_cov_X</code>	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 estimates 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)

Adam Kapelner

 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 $\text{Avg}[|r_{ij}|]$. 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 $\{-1, 1\}^R \times n$ 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_r_ij_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

 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 $\text{Avg}[|r_{ij}|]$. 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 $-1, 1^R \times n$ 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_r_ij_by_R` which is a data frame with $R - R_{\min} + 1$ 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 compute 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 <code>one_zero</code> for 1/0's or <code>pos_one_min_one</code> for +1/-1's.

Value

An matrix of dimension $R \times n$ 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 $n_B * \text{prop}_T$

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 <code>one_zero</code> for 1/0's or <code>pos_one_min_one</code> for +1/-1's.

Value

a matrix where each column is one of the r designs

Author(s)

Adam Kapelner

 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 <code>one_zero</code> for 1/0's or <code>pos_one_min_one</code> for +1/-1's.

Value

a matrix where each column is one of the `r` designs

Author(s)

Adam Kapelner

 initBinaryMatchExperimentalDesignSearch

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

```
initBinaryMatchFollowedByGreedyExperimentalDesignSearch
```

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

<code>X</code>	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.
<code>diff_method</code>	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.
<code>compute_dist_matrix</code>	The function that computes the distance matrix between every two observations in <code>X</code> , its only argument. The default is NULL signifying euclidean squared distance optimized in C++.
<code>...</code>	Arguments passed to <code>initGreedyExperimentalDesignObject</code> . It is recommended to set <code>max_designs</code> 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

`initBinaryMatchFollowedByRerandomizationDesignSearch`

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

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.

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

```
initGreedyExperimentalDesignObject
```

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",
  indices_pairs = NULL,
  Kgram = NULL,
```

```

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

```

Arguments

<code>X</code>	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 <code>Kgram</code> parameter must be specified.
<code>nT</code>	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 <code>X</code> (or <code>Kgram</code> if <code>X</code> is unspecified).
<code>max_designs</code>	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 <code>stopSearch</code> method
<code>objective</code>	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".
<code>indicies_pairs</code>	A matrix of size $n/2$ times 2 whose rows are indicies pairs. The values of the entire matrix must enumerate all indicies $1, \dots, n$. The default is NULL meaning to use all possible pairs.
<code>Kgram</code>	If the <code>objective = kernel</code> , 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.
<code>wait</code>	Should the R terminal hang until all <code>max_designs</code> vectors are found? The default is FALSE.
<code>start</code>	Should we start searching immediately (default is TRUE).
<code>max_iters</code>	Should we impose a maximum number of greedy switches? The default is Inf which a flag for "no limit."
<code>semigreedy</code>	Should we use a fully greedy approach or the quicker semi-greedy approach? The default is FALSE corresponding to the fully greedy approach.
<code>diagnostics</code>	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).
<code>num_cores</code>	The number of CPU cores you wish to use during the search. The default is 1.
<code>seed</code>	The set to set for deterministic output. This should only be set if <code>num_cores = 1</code> 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)
```

```
initGreedyMultipleKernelExperimentalDesignObject
```

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 \mathcal{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

<code>X</code>	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.
<code>max_designs</code>	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 <code>stopSearch</code> method
<code>objective</code>	The method used to aggregate the kernel objective functions together. Default is "added_pct_reduction".
<code>kernel_pre_num_designs</code>	How many designs per kernel to run to explore the space of kernel objective values. Default is 2000.
<code>kernel_names</code>	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 <code>Kgrams</code> parameter.
<code>Kgrams</code>	A list of $M \geq 1$ elements where each is a $n \times n$ 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 <code>kernel_names</code> .
<code>maximum_gain_scaling</code>	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 <code>kernel_pre_num_designs</code> still has $1/1.1 = 9\%$ room to grow making it highly unlikely that any design could be $\geq 100\%$.
<code>kernel_weights</code>	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.
<code>wait</code>	Should the R terminal hang until all <code>max_designs</code> vectors are found? The default is FALSE.
<code>start</code>	Should we start searching immediately (default is TRUE).
<code>max_iters</code>	Should we impose a maximum number of greedy switches? The default is Inf which a flag for "no limit."
<code>semigreedy</code>	Should we use a fully greedy approach or the quicker semi-greedy approach? The default is FALSE corresponding to the fully greedy approach.
<code>diagnostics</code>	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.
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 = 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

<code>X</code>	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 karp design.
<code>wait</code>	Should the R terminal hang until all <code>max_designs</code> vectors are found? The default is FALSE.
<code>balanced</code>	Should the final vector be balanced? Default and recommended is TRUE.
<code>start</code>	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

<code>X</code>	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.
<code>objective</code>	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.

Value

An object of type optimal_experimental_design_search which can be further operated upon

Author(s)

Adam Kapelner

initRerandomizationExperimentalDesignObject
Begin a Rerandomization Search

Description

This method creates an object of type rerandomization_experimental_design and will immediately initiate a search through $S_1 \times T$ 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

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.

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 <code>complete_randomization_with_forced_balanced</code> 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 <code>stopSearch</code> 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 <code>objective = kernel</code> , 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 <code>max_designs</code> 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 <code>num_cores = 1</code> 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, ...)
```

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

Author(s)

Adam Kapelner

`plot.greedy_multiple_kernel_experimental_design`*Plots a summary of a greedy_multiple_kernel_experimental_design object*

DescriptionPlots a summary of a `greedy_multiple_kernel_experimental_design` object**Usage**

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

Arguments

<code>x</code>	The <code>greedy_multiple_kernel_experimental_design</code> object to be summarized in the plot
<code>...</code>	Other parameters to pass to the default plot function

ValueAn 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 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)

Adam Kapelner

```
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)

Adam Kapelner

```
print.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'
print(x, ...)
```

Arguments

x	The binary_then_rerandomization_experimental_design object to be summarized in the console
...	Other parameters to pass to the default print function

Author(s)

Adam Kapelner

```
print.greedy_experimental_design_search
      Prints a summary of a greedy_experimental_design_search ob-
      ject
```

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)

Adam Kapelner

```
print.greedy_multiple_kernel_experimental_design
    Prints a summary of a greedy_multiple_kernel_experimental_design
    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

<code>x</code>	The <code>greedy_multiple_kernel_experimental_design</code> object to be summarized in the console
<code>...</code>	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

<code>x</code>	The <code>karp_experimental_design_search</code> object to be summarized in the console
<code>...</code>	Other parameters to pass to the default print function

Author(s)

Adam Kapelner

```
print.optimal_experimental_design_search
      Prints a summary of a optimal_experimental_design_search ob-
      ject
```

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
      Prints a summary of a pairwise_matching_experimental_design_search
      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)

Adam Kapelner

```
print.rerandomization_experimental_design_search
    Prints a summary of a rerandomization_experimental_design_search
    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 summarized 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 currently 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)

Adam Kapelner

`resultsBinaryMatchThenGreedySearch`*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

<code>obj</code>	The <code>binary_then_greedy_experimental_design</code> object where the pairs are computed.
<code>num_vectors</code>	How many random allocation vectors you wish to return. The default is <code>NULL</code> indicating you want all of them.
<code>compute_obj_vals</code>	Should we compute all the objective values for each allocation? Default is <code>FALSE</code> .
<code>form</code>	Which form should it be in? The default is <code>one_zero</code> for 1/0's or <code>pos_one_min_one</code> for +1/-1's.

Author(s)

Adam Kapelner

`resultsBinaryMatchThenRerandomizationSearch`*Returns unique allocation vectors that are binary matched*

Description

Returns unique allocation vectors that are binary matched

Usage

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

Arguments

obj	The <code>binary_then_greedy_experimental_design</code> 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 <code>one_zero</code> for 1/0's or <code>pos_one_min_one</code> 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 <code>greedy_experimental_design</code> 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 <code>one_zero</code> for 1/0's or <code>pos_one_min_one</code> 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 = 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)

Adam Kapelner

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
design
#how far have we come of the 1000 we set out to do?
ged
#we can cut it here
stopSearch(ged)

## End(Not run)
```

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.
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

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

Description

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

Usage

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

Arguments

obj	The rerandomization_experimental_design object that is currently running the search
include_assignments	Do we include the assignments (takes time) and default is FALSE.
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)

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

X The n x p design matrix

Value

The n x p design matrix with columns standardized

Author(s)

Adam Kapelner

startSearch	<i>Starts the parallelized greedy design search.</i>
-------------	--

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	<i>Stops the parallelized greedy design search.</i>
------------	---

Description

Once stopped, it cannot be restarted.

Usage

```
stopSearch(obj)
```

Arguments

obj	The experimental_design object that is currently running the search
-----	---

Author(s)

Adam Kapelner

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)

Adam Kapelner

```
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 summarized 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 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)

Adam Kapelner

summary.greedy_multiple_kernel_experimental_design

Prints a summary of a greedy_multiple_kernel_experimental_design 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 summarized 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 console
...	Other parameters to pass to the default summary function

Author(s)

Adam Kapelner

```
summary.optimal_experimental_design_search
      Prints a summary of a optimal_experimental_design_search ob-
      ject
```

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
      Prints a summary of a pairwise_matching_experimental_design_search
      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 summarized in the console
...	Other parameters to pass to the default summary function

Author(s)

Adam Kapelner

```
summary.rerandomization_experimental_design_search
```

```
Prints a summary of a rerandomization_experimental_design_search  
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 summarized in the console
...	Other parameters to pass to the default summary function

Author(s)

Adam Kapelner

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