Package ‘minMSE’

April 23, 2020

Type Package
Title Implementation of the minMSE Treatment Assignment Method for One or Multiple Treatment Groups
Version 0.3.1
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Description Performs treatment assignment for (field) experiments considering available, possibly multivariate and continuous, information (covariates, observable characteristics), that is: forms balanced treatment groups, according to the minMSE-method as proposed by Schneider and Schlather (2017) <DOI:10419/161931>.
URL http://www.sebastianschneider.eu
License GNU General Public License
Encoding UTF-8
LazyData true
Imports MASS
NeedsCompilation no
Repository CRAN
Date/Publication 2020-04-23 16:20:02 UTC

R topics documented:

assign_minMSE_treatment .................................................. 2
assign_treatment ................................................................. 5
count_occurrences ............................................................. 8
evaluate_solution ............................................................... 9
evaluate_solution.optim ......................................................... 10
gcd .......................................................... 11
plotting_file ................................................................. 11
program_output ............................................................... 12
sample_with_prev_treatment ................................................ 12
scale_vars ................................................................. 13
assign_minMSE_treatment

minMSE Treatment Assignment for One or Multiple Treatment Groups
    – Wrapper

Description

Calling assign_treatment, this user-friendly wrapper function computes a given number of treatment assignment vectors that will contain at most a certain percentage of duplicates, specified in percentage_equal_treatments. This is useful if non-parametric inference (randomization inference, sometimes called Fisher’s exact test or permutation test) is desired (which is often advised), for analysis of significance of the treatment effect. The main function, assign_treatment, computes the treatment assignment vector according to available data (observable characteristics, covariate vectors) given about the units (individuals or clusters, such as schools, hospitals, ...)

Usage

assign_minMSE_treatment(data, 
    prev_treatment = NULL, 
    n_treatments = 1, 
    n_per_group = NULL, 
    mse_weights = NULL, 
    iterations = 50, 
    change = 3, 
    cooling = 1, 
    t0 = 10, 
    tmax = 10, 
    built_in = 0, 
    desired_test_vectors = 100, 
    percentage_equal_treatments = 1, 
    plot = 0, 
    trace_output = 1, 
    filename = NULL)

Arguments

data a dataframe or a matrix containing the covariate vectors for each attribute. The values might be missing or on different scales as the software deals with missing values and scaling automatically.

prev_treatment takes a numerical vector of partial treatment assignment as argument, and assigns the missing units (where the value is NA) to a treatment group while minimizing the objective function. Non-missing values are copied to the new vector,
assign_minMSE_treatment

i.e., treatment group assignment of these observations is unaffected, but taken into consideration for achieving balanced treatment groups.

\textbf{n_treatments} specifies the number of treatment groups desired (in addition to the control group); minimum and default value is \( n_{\text{treatments}} = 1 \).

\textbf{n_per_group} specifies a vector containing uneven sizes for the treatment groups. Default value is NULL, which yields even sized groups. The sum of the elements in the vector should be equal to the total number of observations.

\textbf{mse_weights} a vector containing the mse_weights for each treatment, or a matrix containing the mse_weights for treatments and outcomes and scaling factors.

\textbf{iterations} specifies the number of iterations the algorithm performs; the default value is \( \text{iterations} = 50 \). Depending on the number of units and the number of covariates to consider for group assignment, a high value could result in a long run-time.

\textbf{change} sets the number of units to exchange treatment in each iteration; the default value is \( \text{change} = 3 \). In case of big datasets (e.g. with more than 100 units), one might consider increasing the default value.

\textbf{cooling} specifies the cooling scheme for the simulated annealing algorithm to use. Cooling = 1, which is the default scheme, sets the temperature to

\[ t_0 / \log(floor((k - 1) / t_{\text{max}}) \times t_{\text{max}} + \exp(1)) \],

whereas cooling = 2 sets the temperature to the faster decreasing sequence

\[ t_0 / (floor((k - 1) / t_{\text{max}}) \times t_{\text{max}} + 1) \].

In praxis, cooling schemes are mostly of one of these forms. One might want to change the cooling scheme if the plot indicates a too slow decrease of objective values. For a theoretical discussion of cooling schemes Belisle (see 1992, p. 890).

\textbf{t0} sets the starting temperature for the simulated annealing algorithm, see Belisle (1992) for theoretical convergence considerations. In praxis, a lower starting temperature \( t_0 \) decreases the acceptance rate of a worse solution more rapidly. Specifying a negative number allows values proportional to the objective function, i.e. \( t_0 = -5 \) sets the starting temperature to \( 1/5 \) of the objective function for the starting point, and thus - for the first \( t_{\text{max}} \) iterations of the algorithm - the difference of the old and the proposed solution is scaled by \( 1/5 \). When changing the default value, it should be considered that also worse solutions have to be accepted in order for the algorithm to escape a local minimum, so it should be chosen high enough. The default value is \( t_0 = 10 \).

\textbf{tmax} specifies the number of function evaluations at each temperature: For instance, \( t_{\text{max}} = 10 \) makes the algorithm evaluate 10 treatment assignments that are found based on the current solution, before the temperature is decreased and thus the probability of accepting a worse solution is decreased. The default value is \( t_{\text{max}} = 10 \).

\textbf{built_in} if \( \text{built}_\text{in} = 1 \) the R built-in function \textbf{optim} with method \textquote{SANN} (Simulated \textit{AN}Nealing) will be used to optimize the function. Otherwise, if \( \text{built}_\text{in} = 0 \), our implementation of the simulated annealing will be used. The function \( \text{built}_\text{in} = 0 \) uses our first cooling function and this cannot be changed. To used the second cooling function, set \( \text{built}_\text{in} = 0 \). All the other parameters, such as iterations, change, \( t_0 \), \( t_{\text{max}} \) are taken into account.
desired_test_vectors

specifies the number of treatment assignment vectors that will be produced to perform Fischer’s exact test (sometimes also called permutation test) for assessment of significance of the treatment effect (this, of course, will be done after treatment has been conducted and measurement of the outcome of interest has occurred). The number of possible treatment vectors will not exceed this number. The default value is desired_test_vectors = 100. For small datasets, one might consider increasing it without affecting performance. Note that this will affect your significance level: If desired_test_vectors = 100 and all of them are unique (see ‘percentage_equal_treatments’ below), you can achieve a significance level of at most $p < 0.01\%$. If desired_test_vectors = 1, then the program returns a single vector that can be used for treatment assignment. Note that Fischer’s exact test might still be possible and that alternative treatment vectors might also be produced after treatment has been conducted; yet, it is not sure how many *different* vectors can be produced with a given number of iterations. It is, therefore, good practice to produce the desired number of vectors with treatment assignment. For testing purposes, however, one might want to produce just one vector.

percentage_equal_treatments

the percentage of non-unique treatment vectors that we allow. The default value is percentage_equal_treatments = 1. Note that this will affect your significance level: If desired_test_vectors = 100 and percentage_equal_treatments = 1, you can achieve a significance level of at most $p < 0.01\%$.

plot

can be used to draw a plot showing the value of the objective function for the a percentage of the iterations by setting plot = 1. The default setting is plot = 0, which suppresses the plot.

trace_output

trace_output = 1 prints helpful output such as the current iteration. To avoid the program output to be too cumbersome, a more detailed output is saved in a txt file called program_output.txt.

filename

takes a string that represents the name of the csv file where the possible treatment assignments will be stored. If filename = NULL, then the file will not be saved.

Value

The program returns a dataframe containing all the unique treatments generated by the program. It also outputs the maximum number of iterations that were reached before finding a non-unique vector.

Note

With the default setting of plotting and using the trace output, the program writes to different files. To avoid this, set plot = 0 and trace_output = 0. For the built-in function optim, the trace output is necessary for printing, because we pipe the output of the program to file to obtain the intermediate values of the optimization function.

Author(s)

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References

Schneider and Schlather (2017), Belisle (1992)

See Also

ginv, optim, assign_treatment

Examples

```r
input <- data.frame(c(10, 20, 30, 40, 130, 40, 120, 5, 10, 80),
                     c(2, 6, 2, 8, 1, 10, 9, 8, 7, 5),
                     c(1, 0, 2, 1, 0, 1, 0, 2, 1, 0))
colnames(input) <- c("IQ", "grade_maths", "both_parents")

assign_minMSE_treatment(input,
                         prev_treatment = c(0, NA, NA, NA, 1, NA, NA, NA, NA, NA),
                         n_treatments = 2,
                         mse_weights = c(1, 2),
                         iterations = 100,
                         trace_output = 1,
                         built_in = 0,
                         desired_test_vectors = 100,
                         plot = 0,
                         filename = NULL)
```

Description

Computes the treatment assignment vector according to available data (observable characteristics, covariate vectors) given about the units (individuals or clusters, such as schools, hospitals, ...). Consider using the user-friendly wrapper function `assign_minMSE_treatment`.

Usage

```r
assign_treatment(current_data,
                 prev_treatment = NULL,
                 n_treatments = 1,
                 n_per_group = NULL,
                 mse_weights = NULL,
                 iterations = 50,
                 change = 3,
                 cooling = 1,
                 t0 = 10,
                 tmax = 10,
                 built_in = 0,
                 plot = 0,
                 create_plot_file = 1)
```
Arguments

current_data  a matrix containing the covariate vectors for each attribute. If the values are missing or on different scales, please use assign_minMSE_treatment, which automatically scales the data.

prev_treatment takes a numerical vector of partial treatment assignment as argument, and assigns the missing units (where the value is NA) to a treatment group while minimizing the objective function. Non-missing values are copied to the new vector, i.e., treatment group assignment of these observations is unaffected, but taken into consideration for achieving balanced treatment groups.

n_treatments specifies the number of treatment groups desired (in addition to the control group); minimum and default value is n_treatments = 1.

n_per_group specifies a vector containing uneven sizes for the treatment groups. Default value is NULL, which yields even sized groups. The sum of the elements in the vector should be equal to the total number of observations.

mse_weights a vector containing the mse_weights for each treatment, or a matrix containing the mse_weights for treatments and outcomes and scaling factors.

iterations specifies the number of iterations the algorithm performs; the default value is iterations = 50. Depending on the number of units and the number of covariates to consider for group assignment, a high value could result in a long run-time.

change sets the number of units to exchange treatment in each iteration; the default value is change = 3. In case of big datasets (e.g., with more than 100 units), one might consider increasing the default value.

cooling specifies the cooling scheme for the simulated annealing algorithm to use. cooling = 1, which is the default scheme, sets the temperature to

\[
t_0/\log(floor((k-1)/tmax) + tmax + exp(1)),
\]

whereas cooling = 2 sets the temperature to the faster decreasing sequence

\[
t_0/(floor((k-1)/tmax) + tmax + 1).
\]

In praxis, cooling schemes are mostly of one of these forms. One might want to change the cooling scheme if the plot indicates a too slow decrease of objective values. For a theoretical discussion of cooling schemes, see Belisle (see 1992, p. 890).

t0 sets the starting temperature for the simulated annealing algorithm, see Belisle (1992) for theoretical convergence considerations. In praxis, a lower starting temperature t0 decreases the acceptance rate of a worse solution more rapidly. Specifying a negative number allows values proportional to the objective function, i.e. t0 = -5 sets the starting temperature to 1/5 of the objective function for the starting point, and thus - for the first tmax iterations of the algorithm - the difference of the old and the proposed solution is scaled by 1/5. When changing the default value, it should be considered that also worse solutions have to be accepted in order for the algorithm to escape a local minimum, so it should be chosen high enough. The default value is t0 = 10.
assign_treatment

**tmax** specifies the number of function evaluations at each temperature: For instance, \( tmax = 10 \) makes the algorithm evaluate 10 treatment assignments that are found based on the current solution, before the temperature is decreased and thus the probability of accepting a worse solution is decreased. The default value is \( tmax = 10 \).

**built_in** if \( built_in = 1 \) the R built-in function `optim` with method 'SANN' (Simulated ANNealing) will be used to optimize the function. Otherwise, if \( built_in = 0 \), our implementation of the simulated annealing will be used. The function \( built_in = 0 \) uses our first cooling function and this cannot be changed. To use the second cooling function, set \( built_in = 0 \). All the other parameters, such as iterations, change, \( t_0 \), \( t_{max} \) are taken into account.

**plot** can be used to draw a plot showing the value of the objective function for the a percentage of the iterations by setting \( plot = 1 \). The default setting is \( plot = 0 \), which suppresses the plot.

**create_plot_file** Used to overwrite the plot file, in case there already exists one. It should only be 1 (true) when this method is called without the wrapper `assign_minMSE_treatment`. This method alone is not capable of plotting, but it will create an auxiliary file that contains the information for plotting. To include plotting, use `assign_minMSE_treatment` with `desired_test_vectors = 1`.

**Value**

Returns the current assignment and the mean squared error value for that assignment.

**Note**

With the default setting of plotting and using the trace output, the program writes to different files. To avoid this, set \( plot = 0 \) and \( trace_output = 0 \). For the built-in function `optim`, the trace output is necessary for printing, because we pipe the output of the program to a file to obtain the intermediate values of the optimization function.

**Author(s)**

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**References**

Schneider and Schlather (2017), Belisle (1992)

**See Also**

`ginv`, `optim`
Examples

\[
\text{input} \leftarrow \text{matrix}(1:30, \text{nrow} = 10, \text{ncol} = 3)
\]

\[
\text{assign_treatment(input,}
\]
\[
\text{prev_treatment} = \text{c}(0, \text{NA}, \text{NA}, 1, \text{NA}, \text{NA}, \text{NA}, \text{NA}, \text{NA}, \text{NA}),
\]
\[
\text{n_treatments} = 2,
\]
\[
\text{mse_weights} = \text{c}(1, 2),
\]
\[
\text{iterations} = 100,
\]
\[
\text{built_in} = 0,
\]
\[
\text{plot} = 0)
\]

---

### count_occurrences

**Count of Equal Treatment Vectors**

#### Description

Checks if the treatment vector given as argument already exists in the dataframe, i.e., has been produced by one or more earlier iteration(s).

#### Usage

\[
\text{count_occurrences(df_treatments, curr_treatment)}
\]

#### Arguments

- `df_treatments`: dataframe containing all the discovered treatment vectors.
- `curr_treatment`: treatment vector to be investigated.

#### Value

Returns the number of treatment assignment vectors which are equal to the one being investigated.

#### Author(s)

Sebastian Schneider <sschneider@coll.mpg.de>; <sebastian@sebastianschneider.eu>, Giulia Baldini <giulia.baldini@uni-bonn.de>

#### Examples

\[
\text{df_treatments} \leftarrow \text{data.frame(c}(0, 2, 0, 1, 1, 0, 2, 1, 1, 0),
\]
\[
\text{c}(0, 2, 0, 1, 2, 0, 1, 2, 1, 0),
\]
\[
\text{c}(0, 2, 1, 1, 2, 0, 0, 2, 0, 0))
\]

\[
\text{colnames(df_treatments)} \leftarrow \text{c}(\text{"treatment_iter_1"}, \text{"treatment_iter_2"}, \text{"treatment_iter_3"})
\]

\[
\text{count_occurrences(df_treatments,}
\]
\[
\text{c}(0, 2, 1, 1, 2, 0, 0, 2, 0, 0))
\]
evaluate_solution  
Evaluate MSE Equation

Description

The function computes the mean squared error for a given treatment assignment. More precisely: it computes the mean squared error of the treatment effect estimator resulting from the treatment groups as specified by the argument, the treatment assignment vector. The function uses matrix multiplication and the Moore-Penrose generalized inverse.

Usage

evaluate_solution(par, data, mse_weights = NULL)

Arguments

par: a treatment assignment. The treatment and the data must have the same number of observations (rows).
data: a matrix containing the covariate vectors for each attribute.
mse_weights: a vector containing the mse_weights for each treatment, or a matrix containing the mse_weights for treatments and outcomes and scaling factors.

Value

Returns the mean squared error value for the current treatment assignment.

Author(s)

Sebastian Schneider <sschneider@coll.mpg.de>; <sebastian@sebastianschneider.eu>, Giulia Baldini <giulia.baldini@uni-bonn.de>

References

Schneider and Schlather (2017).

See Also

ginv

Examples

input <- matrix(1:30, nrow = 10, ncol = 3)

evaluate_solution(par = c(0, 1, 1, 1, 0, 0, 0, 0, 0, 0),
input,
mse_weights = c(1, 2))
evaluate_solution.optim

Evaluate MSE Equation (using optim)

Description

This function calls evaluate_solution, but since optim requires fn and gr to have the same parameters, it has two additional ones.

Usage

evaluate_solution.optim(par,
                         data,
                         mse_weights = NULL,
                         change = NULL,
                         prev_index_list = NULL)

Arguments

par  a treatment assignment. The treatment and the data must have the same number of observations (rows).
data a matrix containing the covariate vectors for each attribute.
mse_weights a vector containing the mse_weights for each treatment, or a matrix containing the mse_weights for treatments and outcomes and scaling factors.
change the parameter is only needed for optim, it does not play any role.
prev_index_list the parameter is only needed for optim, it does not play any role.

Value

Returns the mean square error value for the current treatment assignment.

Author(s)

Sebastian Schneider <sschneider@coll.mpg.de>; <sebastian@sebastianschneider.eu>, Giulia Baldini <giulia.baldini@uni-bonn.de>

References

Schneider and Schlather (2017),

See Also

ginv, optim
gcd

Examples
input <- matrix(1:30, nrow = 10, ncol = 3)
evaluate_solution.optim(par = c(0, 1, 1, 1, 1, 0, 0, 0, 0, 0),
    input)

gcd

Greatest Common Divisor

Description
Computes the GCD of two numbers.

Usage
gcd(v, t)

Arguments
v first input number.
t second input number.

Value
Computes the GCD of the two given numbers

References
https://rosettacode.org/wiki/Greatest_common_divisor#R

Examples
gcd(6, 12)

plotting_file
CSV File for Saving the Data to Plot

Description
CSV file for saving the data to plot.
**Sample with Previous Treatment**

**Description**

File .txt that contains additional output information.

---

**Sample with Previous Treatment**

*Sample Under Consideration of an Already Treated Subset of Units*

**Description**

Given a previous treatment assignment vector for a subset of all observations that treatment assignment is desired for, the function computes a treatment assignment vector for which the previously assigned units are not changed. At a later step, the previously assigned units are also taken into consideration for computation of the score value, the min MSE function, to achieve balanced treatment groups.

**Usage**

```r
sample_with_prev_treatment(prev_treatment, n_treatments, n_per_group)
```

**Arguments**

- `prev_treatment`: takes a numerical vector of partial treatment assignment as argument, and – for a start – assigns the missing units (where the value is NA) to a random treatment group, while maintaining the same proportions in the groups.
- `n_treatments`: specifies the number of treatment groups desired (in addition to the control group). They might be more than the ones already defined in `prev_treatment`.
- `n_per_group`: specifies the distribution of participants per experimental group. It is either an integer, which produces even-sized groups, or a vector which has the same length as the number of experimental groups.

**Value**

Returns a treatment assignment vector where the observations given by `prev_treatment` are unmodified, and the others are assigned to a group.

**Author(s)**

Sebastian Schneider <sschneider@coll.mpg.de>, <sebastian@sebastianschneider.eu>, Giulia Baldini <giulia.baldini@uni-bonn.de>
Examples

    sample_with_prev_treatment(prev_treatment = c(0, NA, NA, 1, NA, NA, NA, NA, NA),
        n_treatments = 2,
        n_per_group = c(2, 4, 4))

scale_vars  Covariate Vectors Scaling

Description

Scales the data such that the empty fields (NA) are the mean of the column and all variables are scaled to have variance 1. In case a variable has zero variance, the variable internally is treated as if it was 0, that way it is not taken into account for treatment assignment.

Usage

    scale_vars(data)

Arguments

data  a dataframe containing the covariate vectors for each attribute.

Value

Returns a dataframe where the empty fields are filled with the mean of the column, and for all variables the variance is 1.

Author(s)

Sebastian Schneider <sschneider@coll.mpg.de>; <sebastian@sebastianschneider.eu>, Giulia Baldini <giulia.baldini@uni-bonn.de>

Examples

    input <- data.frame(c(10, 20, 30, 40, 130, 40, 120, 5, 10, 80),
                        c(2, 6, 2, 8, 1, 10, 9, 8, 7, 5),
                        c(1, 0, 2, 1, 0, 1, 0, 2, 1, 0))
    colnames(input) <- c("IQ", "grade_maths", "both_parents")
    scale_vars(input)
swap_treatment

Swap Treatment

Description

Scrambles the elements of the vector and swaps a predefined number of elements. Afterwards, the vector is ordered according to the original ordering and returned.

Usage

\[
\text{swap\_treatment(} \text{current\_treatment,} \text{ change,} \\
\text{ prev\_index\_list = NULL)}
\]

Arguments

- **current\_treatment**
  
  a treatment vector to be changed.

- **change**
  
  number of elements that will be changed in the treatment vector.

- **prev\_index\_list**
  
  index list of the elements that can be changed. The current treatment vector may belong to a previous, unchangeable assignment.

Value

Returns a new treatment vector.

Author(s)

Sebastian Schneider <sschneider@coll.mpg.de>; <sebastian@sebastianschneider.eu>, Giulia Baldini <giulia.baldini@uni-bonn.de>

Examples

\[
\text{swap\_treatment(} \text{current\_treatment = c(0, 2, 0, 1, 0, 2, 1, 1, 0),} \\
\text{ change = 2)}
\]

\[
\text{swap\_treatment(} \text{current\_treatment = c(0, 2, 0, 1, 0, 2, 1, 1, 0),} \\
\text{ change = 2,} \\
\text{ prev\_index\_list = c(1, 2, 3, 4)}
\]
swap_treatment.optim  Swap Treatment (using optim)

Description

This function calls swap_treatment, but since optim requires fn and gr to have the same parameters, it has an additional one.

Usage

```r
swap_treatment.optim(current_treatment, 
  data = NULL, 
  change, 
  prev_index_list = NULL, 
  mse_weights = NULL)
```

Arguments

- `current_treatment` a treatment vector to be changed.
- `data` the parameter is only needed for optim, it does not play any role.
- `change` number of elements that will be changed in the treatment vector.
- `prev_index_list` index list of the elements that can be changed. The current treatment vector may belong to a previous, unchangeable assignment.
- `mse_weights` the parameter is only needed for optim, it does not play any role.

Value

Returns a new treatment vector.

Author(s)

Sebastian Schneider <sschneider@coll.mpg.de>; <sebastian@sebastianschneider.eu>, Giulia Baldini <giulia.baldini@uni-bonn.de>

See Also

optim

Examples

```r
swap_treatment.optim(current_treatment = c(0, 2, 0, 1, 0, 2, 1, 1, 0), 
  change = 2)
```

```r
swap_treatment.optim(current_treatment = c(0, 2, 0, 1, 0, 2, 1, 1, 0), 
  change = 2, 
  prev_index_list = c(1, 2, 3, 4))
```
vector_gcd  
*Vector Greatest Common Divisor*

---

**Description**

Computes the GCD of a vector.

**Usage**

```r
vector_gcd(vec)
```

**Arguments**

- `vec`  
a vector, for which we want to compute the GCD.

**Value**

The GCD of the elements in the given vector.

**Examples**

```r
input = c(3,6,9)
vector_gcd(input)
```
Index

*Topic assignment
  assign_minMSE_treatment, 2
  assign_treatment, 5
  count_occurrences, 8
  evaluate_solution, 9
  evaluate_solution.optim, 10
  sample_with_prev_treatment, 12
  scale_vars, 13
  swap_treatment, 14
  swap_treatment.optim, 15

*Topic gcd
  gcd, 11
  vector_gcd, 16

*Topic mse
  assign_minMSE_treatment, 2
  assign_treatment, 5
  count_occurrences, 8
  evaluate_solution, 9
  evaluate_solution.optim, 10
  sample_with_prev_treatment, 12
  scale_vars, 13
  swap_treatment, 14
  swap_treatment.optim, 15

*Topic optim
  assign_minMSE_treatment, 2
  assign_treatment, 5
  count_occurrences, 8
  evaluate_solution, 9
  evaluate_solution.optim, 10
  sample_with_prev_treatment, 12
  scale_vars, 13
  swap_treatment, 14
  swap_treatment.optim, 15

*Topic treatment
  assign_minMSE_treatment, 2
  assign_treatment, 5
  count_occurrences, 8
  evaluate_solution, 9
  evaluate_solution.optim, 10

  sample_with_prev_treatment, 12
  scale_vars, 13
  swap_treatment, 14
  swap_treatment.optim, 15

*Topic vector
  vector_gcd, 16

assign_minMSE_treatment, 2, 5–7
assign_treatment, 2, 5, 5

count_occurrences, 8

evaluate_solution, 9, 10
evaluate_solution.optim, 10

gcd, 11
ginv, 5, 7, 9, 10

optim, 3–5, 7, 10, 15

plotting_file, 11
program_output, 12

sample_with_prev_treatment, 12
scale_vars, 13
swap_treatment, 14, 15

swap_treatment.optim, 15

vector_gcd, 16