# Package: minMSE (via r-universe)

# September 8, 2024

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<b>Title</b> Implementation of the minMSE Treatment Assignment Method for One or Multiple Treatment Groups			
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<b>Description</b> 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="">.</doi:10419>			
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assign\_minMSE\_treatment

minMSE Treatment Assignment for One or Multiple Treatment Groups
- Wrapper

# **Description**

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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 as-

signs 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.

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. cool-

ing = 1, which is the default scheme, sets the temperature to

$$t0/log(floor((k-1)/tmax) * tmax + exp(1)),$$

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

$$t0/(floor((k-1)/tmax)*tmax+1).$$

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 Belisle (see 1992, p.

890).

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.

t0

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 used the second cooling function, set built\_in = 0. All the other parameters, such as iterations, change, t0, tmax 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.

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#### 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**

assign\_treatment

Min MSE Treatment Assignment

# **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.

6 assign\_treatment

#### Usage

```
assign_treatment(current_data,
                 prev_treatment = NULL,
                 evaluation_function = evaluate_solution,
                 swap_treatment_function = swap_treatment,
                 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.

evaluation\_function

the function used to evaluate the MSE treatment. Default is evaluate\_solution, which does not take into account outcome or treatment weights. Other options are evaluate\_solution\_vector and evaluate\_solution\_matrix.

swap\_treatment\_function

the function used to create new treatments. Default is swap\_treatment. Other options are swap\_treatment\_prev which, given a previous treatment, creates a new treatment assignment that takes the previous one into account.

n\_treatments specifies the number of treatment groups desired (in addition to the control

group); minimum and default value is  $n_{teatments} = 1$ .

specifies a vector containing uneven sizes for the treatment groups. Default n\_per\_group 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.

a vector containing the mse\_weights for each treatment, or a matrix containing mse\_weights

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.

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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

$$t0/log(floor((k-1)/tmax) * tmax + exp(1)),$$

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

$$t0/(floor((k-1)/tmax)*tmax+1).$$

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.

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, t0, tmax 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.

8 count\_occurrences

#### 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)

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

#### References

```
Schneider and Schlather (2017), Belisle (1992)
```

#### See Also

```
ginv, optim
```

#### **Examples**

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

```
count_occurrences(df_treatments, curr_treatment)
```

#### **Arguments**

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

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#### 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**

```
 \begin{array}{c} \text{df\_treatments} < \text{- data.frame}(c(\emptyset,\ 2,\ \emptyset,\ 1,\ 1,\ \emptyset,\ 2,\ 1,\ 1,\ \emptyset), \\ & c(\emptyset,\ 2,\ \emptyset,\ 1,\ 2,\ \emptyset,\ 0,\ 2,\ \emptyset,\ \emptyset), \\ co(\emptyset,\ 2,\ 1,\ 1,\ 2,\ \emptyset,\ \emptyset,\ 2,\ \emptyset,\ \emptyset)) \\ \text{colnames}(\text{df\_treatments}) < \text{- } c(\text{"treatment\_iter\_1"},\ \text{"treatment\_iter\_2"},\ \text{"treatment\_iter\_3"}) \\ \text{count\_occurrences}(\text{df\_treatments}, \\ & c(\emptyset,\ 2,\ 1,\ 1,\ 2,\ \emptyset,\ \emptyset,\ 2,\ \emptyset,\ \emptyset)) \\ \end{array}
```

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(treatment, data, mse_weights = NULL)
```

# **Arguments**

treatment 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 not used, needed for compatibility.

#### 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**

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

# **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.

evaluation\_function

the function used to evaluate the MSE treatment. Default is evaluate\_solution, which does not take into account outcome or treatment weights. Other options are evaluate\_solution\_vector and evaluate\_solution\_matrix.

swap\_treatment\_function

the parameter is only needed for optim, it does not play any role.

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.

evaluate\_solution\_matrix

```
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
```

#### **Examples**

```
evaluate solution matrix
```

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_matrix(treatment, data, mse_weights)
```

#### **Arguments**

treatment 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 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**

evaluate\_solution\_vector

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_vector(treatment, data, mse_weights)
```

#### **Arguments**

treatment 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.

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# Value

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

# Author(s)

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# References

Schneider and Schlather (2017),

#### See Also

ginv

# **Examples**

output\_file

TXT File That Contains Additional Output Information

# **Description**

File .txt that contains additional output information.

plotting\_file

CSV File for Saving the Data to Plot

# **Description**

CSV file for saving the data to plot.

```
sample_with_prev_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 assigment 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

```
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)

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# **Examples**

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scale\_vars

Covariate Vectors Scaling

# Description

Scales the data such that the empty fiels (NA) are the mean of the column and all variables are scaled to have variance 1. In case a variable has cero 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)

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#### **Examples**

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

# **Arguments**

#### 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**

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

```
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

swap\_treatment\_prev 17

#### **Arguments**

current\_treatment

a treatment vector to be changed.

data the parameter is only needed for optim, it does not play any role.

evaluation\_function

the parameter is only needed for optim, it does not play any role.

swap\_treatment\_function

the function used to create new treatments. Default is <a href="mailto:swap\_treatment">swap\_treatment</a>. Other options are <a href="swap\_treatment\_prev">swap\_treatment</a>, given a previous treatment, creates a

new treatment assignment that takes the previous one into account.

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**

swap\_treatment\_prev

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.

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#### Usage

# 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**

vector\_gcd

Vector Greatest Common Divisor

#### **Description**

Computes the GCD of a vector.

# Usage

```
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.

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# Examples

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

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