

# Flexible Global Optimization with Simulated-Annealing

by Kai Husmann, Alexander Lange and Elmar Spiegel

**Abstract** Standard numerical optimization approaches require several restriction. So do exact methods, like the Newton-Raphson or the Nelder-Mead approach appeal for linearity and unimodality of the loss function. One method to relax these assumptions is the Simulated Annealing approach. There the risk of ending in a local optima is reduced. However the standard implementation still need regular parameter spaces and continuous loss functions. Therefore we implemented a version of the Simulated Annealing method that is able to deal with irregular and complex parameter spaces as well as with non-continuous and sophisticated loss functions. Moreover to gain fast but still reliable solution we included steps to shrink the parameter space during the iterations. All these steps are summarized in the R-package [optimization](#), which we will introduce in the following article. Therefore we also included generic and real world applications of our approach.

## Introduction

As early computer-based optimization methods developed contemporaneously with the first digital computers ([Corana et al., 1987](#)), nowadays numerous optimization methods for various purposes are available ([Wegener, 2005](#)). One of the main challenges in Operations Research is therefore to match the optimization problem with a reasonable method. The complexity of the problem thereby qualifies the possible methods. Optimization procedures in general can be distinguished into exact methods and heuristics ([Kirkpatrick et al., 1983](#)). For simple optimization problems, exact methods are often meaningful tools of choice. If all assumptions on model loss and restrictions are met, these methods will obligatorily find the exact solution without need for further parameters. They are the easiest way of solving optimization problems. The *Linear Simplex-Method* ([Dantzig et al., 1959](#)) as an example which only needs the loss-function and optional restrictions as model input. If, however, any of the model assumptions, e.g. linearity or unimodality, is violated, exact methods are unable to solve problems validly. With developing computer power, heuristics like the *Savings-Algorithm* ([Clarke and Wright, 1964](#)) and metaheuristics like *Simulated Annealing* (SA) ([Kirkpatrick et al., 1983](#)) became popular. They enable solving more complex optimization problems. Metaheuristics are a generalization of heuristics with aim to be even more flexible and efficient ([Blum and Roli, 2003](#)) such that they can solve complex optimization problems, like nonlinear problems. Direct search methods like the *Nelder-Mead* (NM) algorithm are comparatively efficient methods which directly converge to the functions optimum and need relatively less settings ([Geiger and Kanzow, 1999](#)). Random search methods are able to cope with multimodal objective functions. Depending on the method of choice, more or less assumptions on the loss function can be neglected on the one hand. On the other hand, heuristics and metaheuristics will always solve problems approximately. Precision of the solution depends on the optimization method and further parameters. There is even no guaranty of approximating the actual optimum since the solution also depends, by contrast to exact methods, on parameterization ([Blum and Roli, 2003](#)). Definition of proper parameters is thus a crucial point of those methods. The complexity of parameterization will by trend increase with flexibility of the method while efficiency tends to decrease. The efficiency and accuracy of such models is strongly sensitive to their parameter specification ([Corana et al., 1987](#)). Heuristics are often programmed for multi-purpose usage such that there is a suitable method for many optimization problems. For complex optimization problems, however, multi-purpose optimizers often fail to find solutions. Furthermore multi-purpose optimizers are usually not suitable or not efficient for highly complex problems like problems with restricted parameter space. Whenever general-purpose optimizers are too restrictive or inflexible to solve a problem properly, specific methods are advantageous. Those offer a lot of variable parameters such that they be parameterized very specific to the optimization problem. They represent the most flexible and the most complex optimization methods ([Blum and Roli, 2003](#)).

SA ([Kirkpatrick et al., 1983](#)) is known to be one of the oldest and most flexible metaheuristic method, though the term metaheuristic was established after initial publication of SA ([Blum and Roli, 2003](#)). It is known to be favorable against many other methods for multimodal loss functions with a very high number of covariates ([Corana et al., 1987](#)). The method was applied in many studies among several fields covering e.g. chemistry ([Agostini et al., 2006](#)), econometrics ([Ingber, 1993](#)) or forest sciences ([Baskent and Jordan, 2002](#); [Boston and Bettinger, 1999](#)). Since its first implementation by [Kirkpatrick et al. \(1983\)](#), many authors have modified the algorithm in order to adopt it for specific problems (e.g. [DeSarbo et al., 1989](#); [Goffe et al., 1996](#)) or make it more general (e.g. [Xiang et al., 2013](#)). It basically combines systematic and a stochastic components, thus enables escaping local optima. It is

hence typically used for global optimization of multimodal functions. As it offers a lot of options, SA can be named as hybrid method between a general optimizer (when default values are chosen) and a problem specific optimization algorithm (Wegener, 2005). Corana et al. (1987) developed a dynamic adoption method for the variation of the stochastic component during the optimization process. Their modification affects the efficiency as well as the accuracy of the SA algorithm. It has potential to substantially improve the method. Pronzato et al. (1984) suggest to decrease the search-domain of the stochastic component with increasing number of iterations. The stochastic component in general is the most sensitive part of the method since it actually determines the loss variables modification during the iterations.

The R software environment provides platform for simple and effective distribution of statistical models to a huge user community (Xiang et al., 2013). Thus, not surprisingly, several optimization packages of high quality can currently be purchased via *Comprehensive R Archive Network* (Theussl and Borchers, 2016) where even the SA method is recently listed five times. We, however, believe, there is need for a specific stochastic optimization package for complex optimization problems. A package coping with very flexible user definable loss functions with multiple options could be an advantageous extension for R. There is demand for specifically definable optimization problems. We therefore present the package **optimization** which is basically a modified version of SA. We used the properties of SA to program a stochastic optimization method for specific purposes. We therefore focused on flexibility and implemented many user specifiable parameters. Our method is, in its default configuration, usually not immediately efficient on the one but flexibly adoptable to specific purposes on the other hand. Main advantages of the package are the possibilities to specifically adjust covariate changing rules as well as the robustness of the loss function. The changing rule allows the user e.g. to define an integer parameter space. The loss function can return any value, even Na or NaN are possible. Several further user specifications help to parameterize the model problem-specific such that the user can influence accuracy and speed very detailed. It is moreover the first R function where the improvements of Corana et al. (1987) and Pronzato et al. (1984) are implemented into an SA based optimization software. This means, the search domain of the stochastic component of SA dynamically shrinks with increasing iterations. We also implemented a generic plot function for post-hoc inspection of the model convergence assessment and the solution quality. In the following, we briefly introduce the algorithm methodologically and explain the most relevant parameters. We show in four examples where our model is favorable against existing methods and explain how it can be parameterized. We develop two examples illustrating the basic model behavior with focus on the covariate changing rule. Moreover we give hints how to adopt the numerous options to specific problems. Two practical examples where our function is recently used underpin the relevance of our specific-purpose optimization method. One of them, the optimization of forest harvesting schedules is a relatively complex example which cannot be solved with any other optimization function in the R framework.

## The package optimization

In this section, theory of our SA interpretation and resulting parameters are explained.

### Method

Since the basic idea of classic SA is derived from the physical process of metal annealing, the nomenclature of SA comes particularly from metallurgy. Just as the classic SA, our function is composed of an inner for and an outer while loop (Kirkpatrick et al., 1983). The number of iterations in both loops can be defined by the user. For better overview, we displayed the important steps of our function in a pseudocode (Algorithm 1).

### Inner loop

Function of the inner for loop (Algorithm 1, lines 4 to 29) is basically to draw covariate combinations stochastically and to compare the returns. The loop repeats  $n_{inner}$  times. First operation of the inner loop (line 5) is saving the covariate combinations of the last inner iteration as  $x_j$ . In the first iteration  $x_j$  is the vector with user defined initial covariates.

Secondly (line 6), the covariates are changed. This changing process is an essential difference between our approach and the other SA based method in the R framework. Shape and behavior of the variation process may be defined by the user and may be dynamic. Hints and examples for specifying this variation, which is a user defined R function, will be given in the following sections. The variation function  $vf$  is used to create a temporary vector of covariates  $x_{i*}$ . Besides the former covariate combination  $x_j$ , the variation function is allowed to depend on a vector with random factors

$rf$  and the temperature  $t$ . Since  $rf$  and  $t$  change over time, the variation function thus can have dynamic components. Adjustment of  $rf$  and  $t$  is done in the outer loop which will be explained explicitly in the following subsection. In the classical SA approach, the covariates  $x_{i*}$  are generated by adding or subtracting a uniform distributed random number to  $x_j$  (Kirkpatrick et al., 1983). The range of the uniform random number is, in our function, determined by  $rf$  whereas  $rf$  is relative to  $x_j$ . A random factor of 0.1 and a covariate expression of three e.g. leads to a uniform random number between 2.7 and 3.3. This standard variation function is also default in our approach. A very simple exemplary modification of the variation function could e.g. be a normally distributed random number with mean  $x_j$  and standard deviation  $rf$ .

```

1 initialize  $t, rf$  with user specifications
2 calculate  $f(x_0)$  with initial parameter vector  $x_0$ 
3 while  $t > t_{min}$  do
4   for  $i$  in  $c(1: n_{inner})$  do
5      $x_j \leftarrow x_{(i-1)}$ 
6     call the variation function to generate  $x_{i*}$  in dependence of  $x_j, rf$  and  $t$ 
7     check if all entries in  $x_{i*}$  are within the boundaries
8     if all  $x_{i*}$  valid then
9       calculate  $f(x_{i*})$ 
10    else
11      while any( $x_{i*}$  invalid) do
12        call the variation function again
13        count invalid combinations
14      end
15    end
16    if  $f(x_{i*}) < f(x_j)$  then
17       $x_i \leftarrow x_{i*}; f(x_i) \leftarrow f(x_{i*})$ 
18    else
19      calculate Metropolis Probability  $M$  (Equation (1))
20      if uniformly distributed random number  $[0,1] < M$  then
21         $x_i \leftarrow x_{i*}; f(x_i) \leftarrow f(x_{i*})$ 
22      else
23         $x_i \leftarrow x_j; f(x_i) \leftarrow f(x_j)$ 
24      end
25    end
26    if threshold accepting criterion fulfilled then
27      break inner loop
28    end
29  end
30  reduce  $t$  for the next iteration
31   $rf$  adaptation for the next iteration
32 end
33 return optimized parameter vector, function value and some additional information

```

**Algorithm 1:** Pseudocode of the `optim_sa` function in the **optimization** package exemplary for a minimization.

After generating  $x_{i*}$ , the boundaries are checked (lines 7 to 15). If all entries in  $x_{i*}$  are within their respective boundaries, the response is calculated. Otherwise the invalid entries of  $x_{i*}$  are drawn again until all entries are valid. According to Corana et al. (1987), the number of invalid trials can be a useful information to assess quality of the search domain. The numbers of invalid trials are thus counted and stored (line 13) in order to make this information accessible for the outer loop. Counting of valid as well as invalid trials is not reseted after each inner loop repetition. Both are only initialized in iteration one of the inner loop and increase till the last iteration.

Next step is the comparison of loss function returns (lines 16 and 17). If the return of current variables combination  $f(x_{i*})$  is better than  $f(x_j)$ ,  $x_{i*}$  and  $f(x_{i*})$  are stored into  $x_i$  and  $f(x_i)$ , so  $x_i$  are the initial covariates for the next iteration. Core idea of the classical SA approach is to cope with local optima. Thus, even if  $f(x_{i*})$  is worse than  $f(x_j)$ , there is a chance of storing  $x_{i*}$  into  $x_i$  (lines 18 to 25). The likelihood of keeping worse responses depends on the Metropolis probability  $M$  (Metropolis et al., 1953).

$$M = \exp \left( - \frac{|f(i_*) - f(j)|}{kt} \right), \quad (1)$$

with  $k$  being a user definable constant. We adopted this strategy from classic SA without modifications.  $M$  decreases with decreasing temperature  $t$ . The likelihood of keeping worse responses thus decreases

with decreasing temperature  $t$  (lines 19 and 24).  $t$  does not change during the entire inner for loop. The likelihood of keeping worse values is thus equal for each response until the inner loop is finished. Modification of  $t$  is part of the outer loop which will be explained in the next paragraph. In case a worse result is chosen the former optimal covariate combination is, of course, stored before it is overwritten since otherwise there is a sound chance of overwriting that actual global optimum. More details of the Metropolis probability can i.a. be found in [Kirkpatrick et al. \(1983\)](#) and [Metropolis et al. \(1953\)](#).

Storing information on development of covariates and response can help improving the performance of SA ([Lin et al., 1995](#); [Hansen, 2012](#)). We implemented a threshold accepting strategy ([Dueck and Scheuer, 1990](#)) into our SA interpretation (lines 26 to 28). This criterion is the only module that allows reducing the inner loop repetitions without direct user influence. It is simply a vector where the absolute differences of  $f(x_i)$  and  $f(x_j)$  are stored. If the response oscillates for user defined number of repetitions within a user defined threshold, the inner loop breaks.

## Outer loop

Main functions of the outer while loop (lines 3 to 32) are calling the inner loop (lines 3 to 29) and modifying the parameters that are needed in the inner loop (lines 30 and 31). Therefore  $t$  and  $rf$  only change after completely finishing an inner loop. The outer loop repeats till  $t$  is smaller than the user defined minimum temperature  $t_0$ .

After finishing the inner loop, firstly  $t$  is adjusted (line 30).  $t$  is necessary for the stochastic part in the inner loop (line 19, Equation (1)). In our function,  $t$  is obligatory decreasing as it is calculated by multiplying the temperature of the current iteration by  $r$  which is a user defined real number between 0 and 1. The number of outer loops repetitions is thus implied by initial temperature  $t_0$ ,  $t_{min}$  and  $r$ .

Afterwards  $rf$  changes (line 31). The dynamic adaption of  $rf$  after [Corana et al. \(1987\)](#) and [Pronzato et al. \(1984\)](#) is another major novelty of our function. As each covariate can have its own random factor,  $rf$  is a vector of the same size as  $x_i$ .  $rf$  is needed for the covariate variation in the inner loop (lines 6 and 12). Dividing the numbers of invalid trials which were counted in the inner loop (line 13) distinctively for each covariate by the total number of trials of the respective covariate gives the ratio of invalid trials for each covariate. According to ([Corana et al., 1987](#)), this ratio of invalid trials can be used to find a trade-off between accuracy on the one and size of the search domain on the other side. They argument that if only valid covariate combinations are drawn, the search domain could be too small for multimodal problems. For this, the ratio of invalid trials in the current iteration is used to generate the  $rf$  for the following outer loop repetition. They suggest ratios between 0.4 and 0.6. If any observed ratio of invalid trials is  $< 0.4$  or  $> 0.6$ , the respective random factors are modified following the suggested equation by [Corana et al. \(1987\)](#). This strategy allows a adjustment of  $rf$  for the next iteration. [Pronzato et al. \(1984\)](#), who developed the *Adaptive Random Search method*, propose a time decreasing search domain. Thus they suggest a search domain adjustment that does not depend on former information, as [Corana et al. \(1987\)](#) did, but on the number of iterations. They argument that the search domain should be wide at the beginning to give the algorithm the chance of coping local optima and small in the end to allow higher precisions since the algorithm should converge to the global optimum at the end. Later iteration thus need smaller search domains than earlier iterations. We combined the idea of [Pronzato et al. \(1984\)](#) into the dynamically search domain adjustment of ([Corana et al., 1987](#)) by linearly shrinking the favorable range of ratios from the suggested ratios (0.4-0.6) to 0.04-0.06. As mentioned in the inner loop explanations, the variation function can be user defined (lines 6 and 12). The user thus has the chance of defining flexibly in which way  $t$  and  $rf$  influence the covariate variation. Per default, the search domain around the covariates shrinks by trend with increasing number of outer loop iterations.

## The function `optim_sa`

`optim_sa` shall be able to solve very specific optimization problems, several parameters can be defined by the user. Quality of solution and speed of convergence will thus substantially depend on accurate parametrization. In the following, we will explain the most important parameters briefly giving hints for useful specification. A complete parameter list can be found in the vignette.

- `fun`: Obligatory loss function to be optimized. The function must depend on a vector of covariates and return one numeric value. There are no assumptions on covariates and return. The covariates not even need to be continuous. Missing (NA) or undefined (NaN) returns are allowed as well. Any restriction on the parameter space, e.g. specific invalid covariate values within the boundaries, can be integrated in the loss function directly by simply returning NA. We will be more specific on this in the practical examples.

- `start`: Obligatory numeric vector with initial covariate combination. It must be ensured that at least the initial covariate combination leads to a defined numeric response. The loss function at the initial variables combination must therefore return a defined numeric value. This might be relevant when the starting values are determined stochastically.
- `trace`: If `TRUE`, the last inner loop iteration of each outer loop iteration is stored as row in the trace matrix. This might help evaluating the solutions quality. However, storing interim results increases calculation time up to 10 %. Disabling trace can thus improve efficiency when the convergence of an optimization problem is known to be stable.
- `lower, upper`: Numeric vector with lower boundaries of the covariates. The boundaries are obligatory since the dynamic rf adjustment (Corana et al., 1987; Pronzato et al., 1984) depends on the number of invalid covariate combinations.
- `control`: A list with optional further parameters.

All parameters in the list with `control` arguments have a default value. They are pre-parameterized for loss functions of medium complexity. `control` arguments are:

- `vf`: Variation function that allows the user to restrict the parameter space. It is one of the most important differences to classic SA. The function determines the variation of covariates during the iterations. It is allowed to depend on `rf`, `temperature` and the vector of covariates of the current iteration. The variation function is a crucial element of `optim_sa` which enables flexible programming. It is (next to the loss function itself) the second possibility to define restrictions. The parameter space of the optimization program can be defined by `vf`. Per default, the covariates are changed by a continuous, uniform distributed random number. It must be considered that defining specific `rf` can increase the calculation time. The default `rf` is a compiled C++ function whereas user specified `rf` must be defined as R functions. User specified are e.g. useful for optimization problems with non-continuous parameter space.
- `rf`: Numeric vector with random factors. The random factors determine the range of the random number in the variation function `vf` relative to the dimension of the function variables. The `rf` can be stated separately for each variable. Default is a vector of ones. If `dyn_rf` is enabled, the entries in `rf` change dynamically over time.
- `dyn_rf`: Boolean variable that indicates if the `rf` shall change dynamically over time to ensure increasing precision with increasing number of iterations. `rf` determines whether the adjustments of Corana et al. (1987) and Pronzato et al. (1984) are enabled (see method section for theoretical background). `dyn_rf` ensures a relatively wide search domain at the beginning of the optimization process that shrinks over time. Disabling `dyn_rf` can be useful when `rf` with high performance are known. The development of `rf` is documented in the trace matrix. Evaluation of former optimizations with dynamic `rf` can thus help finding efficient and reasonable fixed `rf`. Self-specified `vf` may not depend on `rf`. In this cases activating `dyn_rf` does not change the process.
- `t0`: Initial temperature. The temperature directly influences the likelihood of accepting worse responses thus the stochastic part of the optimization. `t0` should be adopted to the loss function complexity. Higher temperatures lead to higher ability of coping with local optima on the one but also to more time-consuming function calls on the other hand.
- `t_min`: Numeric value that determines the temperature where outer loop stops. As there is practically no chance of leaving local optima in iterations with low temperature `t_min` mainly affects accuracy of the solution. Higher `t_min` yields to lower accuracy and less function calls.
- `nlimit`: Integer value which determines the maximum number of inner loops iterations. If the break criterion in the inner loop is not fulfilled, `nlimit` is the exact number of inner loops repetitions. It is therefore an important parameter for determining the number of iterations.
- `r`: Numeric value that determines the reduction of the temperature at the end of each outer loop. Slower temperature reduction leads to increasing number of function calls. It should be parameterized with respect to `nlimit`. High `nlimit` in combination with low `r` lead to many iterations with the same acceptance likelihood of worse responses. Low `nlimit` in combination with `r` near 1, by contrast, lead to continuously decreasing acceptance likelihood of worse responses. It is thus the second crucial parameter for determining the number of iterations.

## Examples

To show the benefits of our **optimization** package we build four examples explaining where the `optim_sa` function can be advantageous.



**Table 1:** Relative frequencies of covariate combinations in % after optimization for the four examined methods. Number of repetitions: 10,000. We used the parameters given in the example, only the trace options was deactivated.

	Method	Result (rounded)			
		{-2.8, 3.1}	{3.0, 2.0}	{3.6, -1.8}	{-3.8, -3.3}
	optim_sa	22.19	33.49	28.05	16.27
	optim (SA)	25.91	30.89	24.08	19.12
	GenSA	0.00	0.00	0.00	100.00
	optim (NM)	0.00	0.00	0.00	100.00

### Himmelblau Function with continuous parameter space

Himmelblau's function (Equation (2)) (Himmelblau, 1972) was chosen as initial example since it is a very simple multimodal equation which is widely known in Operations Research. It has four equal minimum values ( $\min(f(x_1, x_2)) = 0$ ) at  $\{-2.8, 3.1\}$ ,  $\{3.0, 2.0\}$ ,  $\{3.6, -1.8\}$  and  $\{-3.8, -3.3\}$ . In order to display the basic behavior of **optimization**, it was compared with two other SA methods from the packages **stats** and **GenSA**. Himmelblau's function is relatively simple. Therefore we also included the NM optimization method (Nelder and Mead, 1965) which is default of **optim** from the **stats** package, to examine the advantages of stochastic search against direct search.

$$f(x_1, x_2) = (x_1^2 + x_2 - 11)^2 + (x_1 + x_2^2 - 7)^2 \quad (2)$$

We performed 10,000 repetitions with each function in order investigate quality and speed of the solutions using parameters for relatively simple optimization problems for all examined methods. The optimizations were performed having the following parameters:

```
# stats package: optim (NM)
stats::optim(fn = hi, par = c(10, 10), method = "Nelder-Mead")

# optimization package: optim_sa
optimization::optim_sa(fun = hi, start = (c(10, 10)), trace = TRUE,
  lower = c(-40, -40), upper = c(40, 40),
  control = list(t0 = 500, nlimit = 50, r = 0.85,
    rf = 3, ac_acc = 0.1, dyn_rf = TRUE))

# stats package optim (SA)
stats::optim(fn = hi, par = c(10, 10), method = "SANN",
  control = list(tmax = 500, reltol = 0.1, temp = 50, trace = TRUE))

# GenSA package: GenSA
GenSA::GenSA(fn = hi, par = c(10, 10), lower = c(-40, -40), upper = c(40, 40),
  control = list(temperature = 50, nb.stop.improvement = 30, maxit = 500))
```

Since we have a multimodal optimization problem with multiple equal solutions, evaluation of solutions quality is composed of response accuracy and covariate combination. With fixed starting parameters, the methods should be able to find all possible solutions. We defined the problem to be solved with sufficient accuracy when the response was  $\leq 0.01$ . We also looked at the frequency distribution of the covariate combination after minimization. Subsequent to investigation of quality, we also compared the efficiencies by measuring calculation times using **microbenchmark** and the iterations frequencies.

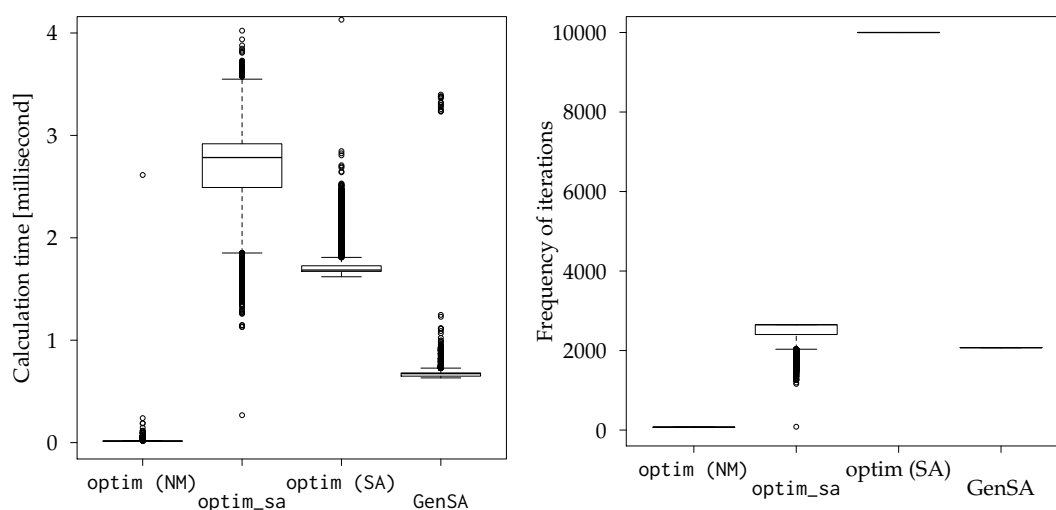
It became clear that parameterization of NM was quite easy. It only needed a vector with starting values. The other functions needed much more settings. With view to accuracy each method performed well. All functions returned in mean of 10,000 calls responses with values  $\leq 0.01$ . With view to frequency distribution, the functions performed different (Table 1). **optim\_sa** and **optim (SA)** returned each possible solutions. The combination  $\{-3.8, -3.3\}$  was consistently least frequent. **GenSA** and **optim (NM)**, however, solely returned  $\{-3.8, -3.3\}$ . Further investigation revealed the solutions of **GenSA** and **optim (NM)** to be sensitive of the starting values. If **GenSA** and **optim (NM)** were parameterized with randomly drawn starting values, all four results would have been possible. Advantage of **optim\_sa** and **optim (SA)** against **GenSA** and **optim (NM)** is, in this example, thus its independence from starting values.

As all functions were practically able to minimize Equation (2), comparison of calculation times appears to be another important point for quality assessment. As expected, the direct search method

optim (NM) was by far faster than all stochastic methods (Figure 1, left). The within-group ranking of stochastic methods revealed GenSA to be fastest. It was in average 3.5 times faster than optim\_sa. The two functions able coping with equally valued optima (optim (SA) and optim\_sa) were slower than GenSA (Table 1; Figure 1, left).

Another way of comparing algorithms efficiency is to examine the frequency of necessary iterations solving the optimization problem. Again, optim (NM) performed best (Figure 1, right). While optim\_sa and GenSA showed in average roughly the same numbers of iterations, optim (SA) needed by far most repetitions. Only optim\_sa showed varying frequencies because optim\_sa was, given the displayed parameters, the only function where the inner loop broke due to the threshold accepting criterion. It could be seen that optim\_sa performed good when compared to established SA based optimization functions. The calculation of valid parameter combinations (Algorithm 1, lines 7 to 15) leads to multiple function calls within one iteration. For this, one iteration of optim\_sa can last longer than one iteration of the other methods. The dyn\_rf which adopts the search domain dynamically to specific loss function on the one hand thus leads to longer calculation times on the other hand. Improved flexibility therefore again corresponds with longer calculation times.

To conclude, all functions were generally able to solve the problem. The flexible stochastic search-grid of optim (SA) and optim\_sa enabled archiving each of the four solutions. Practically, in case users are in doubt whether a problem has multiple solutions with equal responses, optim (SA) and optim\_sa can simply be repeated without re-parameterization. If well-specified, they will return all possible solutions. They are thus advantageous for complex multimodal problems of that kind on the one hand, but slower on the other hand. Due to the multiple additional options, which all have to be called in the code, optim\_sa is slowest. This example clearly reveals that higher flexibility and generality leads to significantly higher calculation times. Specific algorithms are advantageous for complexer problems while more general functions are useful for optimization problems with simple responses.



**Figure 1:** Calculation times and frequency of iterations of the four examined optimization algorithms in Example 1. Note that the y-axis of the left diagram is truncated. optim\_sa sowed 101 and optim (SA) 70 outliers between four and seven milliseconds. The frequency of iterations represents the total number of iterations. thus, for the SA methods, all inner loops repetitions are counted.

### Himmelblau Function with discrete parameter space

A second example illustrating the advantage of flexibly defining the parameter spaces also bases on the function by Himmelblau (1972). It is an exemplary optimization problem which cannot be solved with any other examined method. If a user is interested in integer covariate combinations only, simply rounding the solution is usually not satisfying since the solution could be non-feasible or non-optimal (Cardoso et al., 1997). The flexible variation function vf of our models allows searching for integer temporary solutions only and thus searching for the global integer solution. vf can be used to restrict the parameter space to the specific problem. The following simple example shows a variation rule for an exemplary integer programming problem. The simple var\_fun\_int from the example returns

a vector of integer covariates varying in dimension of `vf` around the passed covariates `para_0`. The `fun_length` must be passed explicitly, although it is implicitly given by the length of `para_0` because it might help simplifying the function `vf`. Dependence of `rf` and `temp` can be implemented. Optimization problems do not always need a dynamic component. If `vf` need not be dynamic, i.e. if the stochastic part shall be fixed during the entire iterations, `temp` and `rf` can separately be disabled by passing `NA` for the respective parameter. If `vf` does not depend on `rf`, the option `dyn_rf` will not be useful any more. It should be disabled in such cases to save computation time.

```
# Define vf
var_fun_int <- function (para_0, fun_length, rf, temp = NA) {
  ret_var_fun <- para_0 + sample.int(rf, fun_length, replace = TRUE) *
    ((rbinom(fun_length, 1, 0.5) * -2) + 1)
  return (ret_var_fun)
}

# Call optim_sa
int_programming <- optimization::optim_sa(fun = hi, start = c(10, 10), trace = TRUE,
  lower = c(-40, -40), upper=c(40, 40),
  control = list(t0 = 500, nlimit = 50,
    r = 0.85, rf = 3, ac_acc = 0.1,
    dyn_rf = TRUE, vf = var_func_int))
```

Calling the minimization function times led to the only integer solution {3, 2}. The generic plot function of optimization (Figure 2) helps interpreting the convergence and thus the solution quality as well as the algorithm behavior. Since the example is 2-dimensional, a contour\_plot (Figure 2, right) could be created. It shows the state space of the Himmelblau function in continuously changing colors for parameter spaces between -4 and 4. The results at the end of each outer loop iteration are shown as points within the parameter space. It became obvious that only integer covariate combinations were calculated during the entire optimization (Figure 2, right). Figure 2 additionally helps explaining the stochastic part of the SA method. It becomes clear that though response of iteration 10 (parameter combination {0, 0}) was already quite near 0, following iteration ended with a relatively worse intermediate results. With response > 100, iteration 19 (parameter combination {2, 3-}) was much worse than iteration 12. The likelihood of keeping worse solutions shrank over time till it became practically 0 after iteration 40 (Figure 2, left). For problems of such kind, 40 iterations therefore should be far enough. This information could help the user parameterizing the function for the next problem.

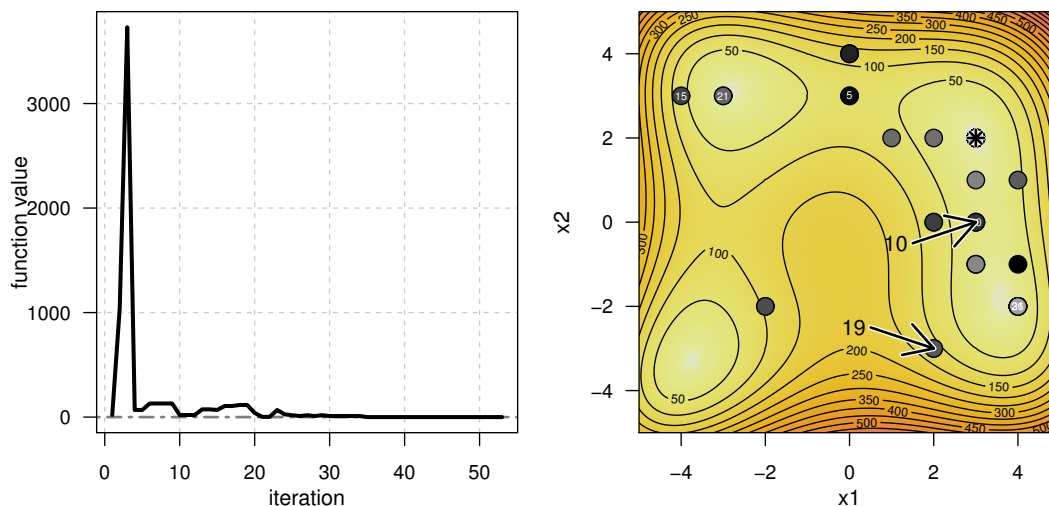
`optim` (SA) also provides possibility of defining a variation function via the `gr`. Using the variation function from the example code with fixed `rf`, however, it was not possible to define robust parameters for solving an integer programming problem. `optim_sa` is thus advantageous against all other examined functions when the parameter space of the optimization problem underlies extended restrictions. It is the only function that enables global optimum integer search. To archive this, the user must define a changing rule in form of a R function. Users must thus examine their optimization problem very carefully and translate it into suitable functions. Parameterization of `optim_sa` is quite complex and time extensive but enables adopting the optimizer to problem specific needs. Other restrictions such as mixed integer problems may be defined analogously. `vf` can thus be used to flexibly restrict the parameter space. Further hints for interpretation can be found in the package documentation.

## Structural vector autoregressive models with least dependent innovations

*Vector autoregressive* (VAR) models are used to examine dynamic structures of several time series endogenously within one model. Usually, impulse response functions come to use for investigating the between-series relationships. Those compositions, however, are not unique. The interactions between the time series variables in a VAR model are hence not directly calculable. The idea behind *structural* VAR (SVAR) is to define strategies to overcome the problem and enable unique impulse response definitions (Lütkepohl, 2006).

Least dependent innovations is one of plenty possibilities to obtain unique decompositions of the covariance matrix. It is one strategy to generate unique orthogonalized impulse responses in a VAR model. The idea is to minimize a Cramer-von-Mises test statistic for stochastically independent structural errors (Genest et al., 2007). Basically, a vector of  $K(K-1)/2$  rotation angles between 0 and  $2\pi$ , is modified until the stochastically independent structural errors become minimal.  $K$  is the number of time series in the SVAR model. Alex, an dieser Stelle koenntest Du in 1-2 Satzen sagen, mit womit der Vector multipliziert wird. An advantage of this method is, that it is very liberal in sense of distribution assumptions (Herwartz, 2014).





**Figure 2:** Exemplary examination plots created with the generic plot function. The left diagram shows the current optimal response over iteration of the outer loop. The left diagram displays the succession of the covariate values. The star points the covariate combination at optimum. The actual parameter space of the optimization is reduced for presentation reasons.

However, optimizing the test statistic is challenging, because the loss function has a large and unpredictable number of local optima and an irregular state space. Moreover, the function shows a relatively broad parameter space with very sensitive responses. It often reacts dramatically to small changes in the rotation angles. One approach to solve the optimization problem is the *grid optimization* (Herwartz and Plödt, 2015). Grid optimization is, however, inefficient in large samples and – depending on the step size – sometimes unable to find the global optimum. Monte Carlo simulations have shown that direct search and gradient based optimization algorithms usually fail to find the optimal rotation angles. Performing several direct search optimizations sequentially with randomly changing starting values can lead to satisfying solutions. The strategy is, however, also very inefficient.

The irregular response pattern and the high demands on the solution precision are the main challenges. The combination of SA with the adaptive variation of the search seems to be promising for the optimization problem. The relatively broad parameter variation at the beginning of the optimization process should ensure adequate search-grid size while the stochastic component of the SA should be able to tackle the irregular responses. Dynamically decreasing parameter variation is particularly advantageous for optimizing the rotation angles as sufficient parameter accuracy is crucial for the reliability of the solution.

Practical application of `optim_sa` revealed its advantages. Using parameterizations for low performance and high precision, e.g. an initial temperature of 100,000, a maximum number of 10,000 inner loops and temperature reductions between 0.7 and 0.9, it was still more efficient than all other investigated methods. Sensitivity analysis of exemplary optimization problems confirmed the general applicability of `optim_sa`. The function was able to find the actual global optimum sufficiently often.

### Forest harvesting schedule optimization

Forestry is traditionally knowledge-based field with optimization playing only minor role. However popularity of optimization methods is steadily rising. While Linear Programs are nowadays used in some states, e.g. Finland (Redsven et al., 2012), stochastic optimization programs are quite novel in forestry for optimization of harvesting intensity (Kangas et al., 2015). Our function is integral part of the first stochastic optimization software of forest operation in Germany and one of the first softwares worldwide on single tree scale. Optimization of forest harvesting planning represents an interesting and innovative practical example where `optim_sa` is recently used. `optimization` is part of the Forest Planner based decision support software for forest enterprises by Hansen and Nagel (2014). Forest Planner is a user front end for *Tree Growth Open Source Software* (TreeGrOSS) which is a complex Java written tree growth and yield simulation software used to forecast the developments of forest management areas (stands). It is a tool able to simulate forest enterprises with hundreds of forest stands simultaneously where the smallest simulation element is the single tree. Each tree in the system is thus simulated individually. Optimization of forest activities is accordingly not trivial

since TreeGrOSS is a complex network of rules and functions which are predominantly nonlinear. The entire optimization process is composed of TreeGrOSS, **optimization** and a data warehouse. This multi-factorial composition implies high demand for flexibility of the optimization function. Loss function, which represents in this example the interface between the three elements of the optimization system, must be composed of R, Java (using **rJava**) and SQL (using **RPostgreSQL**). Main tasks of the interface are enabling communication between TreeGrOSS and optimization algorithm and rating the TreeGrOSS output in terms of costs and revenue such that the TreeGrOSS output is translated into a response readable by the optimization algorithm. Flexibility of loss and variation functions is hence a prerequisite for forest harvesting schedule optimization via TreeGrOSS simulations. Each loss function call causes a TreeGrOSS simulation and a database operation. In order to save time, parts of the loss are therefore programmed parallel. The response is, accordingly, nonlinear and particularly non-continuous. Random search methods are of therefore favorable for the problem. Obligatory sustainability of forest stand treatment is also considered in form of restrictions. Each function call returns, next to the actual response, a sustainability index. This index is used to restrict the optimization by simply defining NA responses whenever sustainability is violated.

It showed that forest treatment optimization was actually possible using **optimization**. We developed a loss function able translating the TreeGrOSS in- and output into interpretable variables for `optim_sa`. Sensitivity analysis using an exemplary forest enterprise comprised of five forest stands, with known global maximum, reinforced reliability of `optim_sa` for harvesting optimization. A solution sufficiently near the global maximum was found in arguable time on a standard personal computer. To test the practical usability, the optimization system was additionally tested on a real forest enterprise with 100 forest stands. The problem was solved within twelve hours using a cluster computer. Repeating the optimization three times led to equal responses but different harvesting volumes (thus covariate combinations). This again reveals the complexity of the problem and further reinforces the need for specific stochastic methods.

## Discussion and outlook

All in all SA methods are advantageous compared to classical optimization procedures, if the loss function is non-linear and multimodal. Our simulated annealing approach optimizes these functions quite well. It might not be faster than the standard simulated annealing approach of the **stats** package, but therefore it was not designed. However, due to the shrinkage of the parameter space and the extra stopping criteria it manages to need less steps than the standard approach. Moreover the main advantage of our new approach is to be able to deal with irregular parameter spaces, as well as with non-continuous and sophisticated loss functions, where the standard approach reaches its limits. In our examples we show that problems with these characteristics exist and that our algorithm solves these problems. Furthermore there are several examples of loss functions in natural science where some combinations of variables are restricted and our approach shows its benefits.

## Bibliography

- F. P. Agostini, D. D. O. Soares-Pinto, M. A. Moret, C. Osthoff, and P. G. Pascutti. Generalized simulated annealing applied to protein folding studies. *Journal of computational chemistry*, 27(11):1142–1155, 2006. [p1]
- E. Z. Baskent and G. A. Jordan. Forest landscape management modeling using simulated annealing. *Forest Ecology and Management*, 165(1):29–45, 2002. [p1]
- C. Blum and A. Roli. Metaheuristics in combinatorial optimization: Overview and conceptual comparison. *ACM Computing Surveys (CSUR)*, 35(3):268–308, 2003. [p1]
- K. Boston and P. Bettinger. An analysis of monte carlo integer programming, simulated annealing, and tabu search heuristics for solving spatial harvest scheduling problems. *Forest science*, 45(2):292–301, 1999. [p1]
- M. F. Cardoso, R. Salcedo, S. F. de Azevedo, and D. Barbosa. A simulated annealing approach to the solution of minlp problems. *Computers & chemical engineering*, 21(12):1349–1364, 1997. [p7]
- G. Clarke and J. W. Wright. Scheduling of vehicles from a central depot to a number of delivery points. *Operations research*, 12(4):568–581, 1964. [p1]
- A. Corana, M. Marchesi, C. Martini, and S. Ridella. Minimizing multimodal functions of continuous variables with the “simulated annealing” algorithm. *ACM Trans. Math. Softw.*, 13(3):262–280, 1987. [p1, 2, 3, 4, 5]

- G. B. Dantzig, D. R. Fulkerson, and S. M. Johnson. On a linear-programming, combinatorial approach to the traveling-salesman problem. *Operations Research*, 7(1):58–66, 1959. [p1]
- W. S. DeSarbo, R. L. Oliver, and A. Rangaswamy. A simulated annealing methodology for clusterwise linear regression. *Psychometrika*, 54(4):707–736, 1989. [p1]
- G. Dueck and T. Scheuer. Threshold accepting: a general purpose optimization algorithm appearing superior to simulated annealing. *Journal of computational physics*, 90(1):161–175, 1990. [p4]
- C. Geiger and C. Kanzow. Das nelder-mead-verfahren. *Numerische Verfahren zur Lösung unregistrierter Optimierungsaufgaben*, 1999. [p1]
- C. Genest, J.-F. Quessy, and B. Remillard. Asymptotic local efficiency of cramer-von mises tests for multivariate independence. *The Annals of Statistics*, 2007. [p8]
- W. L. Goffe et al. Simann: A global optimization algorithm using simulated annealing. *Studies in Nonlinear Dynamics and Econometrics*, 1(3):169–176, 1996. [p1]
- J. Hansen and J. Nagel. *Waldwachstumskundliche Softwaresysteme auf Basis von TreeGrOSS: Anwendung und theoretische Grundlagen*. Beiträge aus der Nordwestdeutschen Forstlichen Versuchsanstalt / Nordwestdeutsche Forstliche Versuchsanstalt. - Göttingen : Univ.-Verl. Göttingen, 2007- ; 11Universitätsdrucke Göttingen. Univ.-Verl., Göttingen, 2014. ISBN 978-3-86395-149-8. [p9]
- J. H. Hansen. *Modellbasierte Entscheidungsunterstützung für den Forstbetrieb: Optimierung kurzfristiger Nutzungsoptionen und mittelfristiger Strategien unter Verwendung metaheuristischer Verfahren und parallelen Rechnens*. Cuvillier, Göttingen, 1. aufl. edition, 2012. [p4]
- H. Herwartz. Structural analysis with independent innovations. *cege Discussion Papers*, 2014. [p8]
- H. Herwartz and M. Plödt. The macroeconomic effects of oil price shocks: Evidence from a statistical identification approach. *Journal of International Money and Finance*, 2015. [p9]
- D. M. Himmelblau. *Applied nonlinear programming*. McGraw-Hill Companies, 1972. [p6, 7]
- L. Ingber. Simulated annealing: Practice versus theory. *Mathematical and computer modelling*, 18(11):29–57, 1993. [p1]
- A. Kangas, M. Kurttila, T. Hujala, K. Eyvindson, and J. Kangas. *Decision Support for Forest Management*. Number 30 in Managing Forest Ecosystems. Springer International Publishing, Cham, 2nd ed edition, 2015. [p9]
- S. Kirkpatrick, C. D. Gelatt, M. P. Vecchi, et al. Optimization by simulated annealing. *science*, 220(4598):671–680, 1983. [p1, 2, 3, 4]
- C. Lin, K. Haley, and C. Sparks. A comparative study of both standard and adaptive versions of threshold accepting and simulated annealing algorithms in three scheduling problems. *European Journal of Operational Research*, 83(2):330–346, 1995. [p4]
- H. Lütkepohl. Structural vector autoregressive analysis for cointegrated variables. In *Modern Econometric Analysis*, pages 73–86. Springer, 2006. [p8]
- N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller. Equation of state calculations by fast computing machines. *The journal of chemical physics*, 21(6):1087–1092, 1953. [p3, 4]
- J. Nelder and R. Mead. A simplex method for function minimization. *Computer Journal*, 7(4):308–313, 1965. [p6]
- L. Pronzato, E. Walter, A. Venot, and J.-F. Lebruchec. A general-purpose global optimizer: Implimentation and applications. *Mathematics and Computers in Simulation*, 26(5):412–422, 1984. ISSN 03784754. doi: 10.1016/0378-4754(84)90105-8. [p2, 4, 5]
- V. Redsven, H. Hirvelä, K. Härkönen, O. Salminen, and M. Siitonen. *MELA2012 Reference Manual (2nd edition)*. The Finnish Forest Research Institute, 2012. [p9]
- S. Theussl and H. W. Borchers. CRAN Task View: Optimization and Mathematical Programming. Oct. 2016. URL <https://CRAN.R-project.org/view=Optimization>. [p2]
- I. Wegener. Simulated annealing beats metropolis in combinatorial optimization. In *International Colloquium on Automata, Languages, and Programming*, pages 589–601. Springer, 2005. [p1, 2]

Y. Xiang, S. Gubian, B. Suomela, and J. Hoeng. Generalized simulated annealing for global optimization: the gensa package. *The R Journal Volume 5(1):13-29, June 2013, 2013*. [p1, 2]

*Author One*

*Affiliation*

*Address*

*Country*

author1@work

*Author Two*

*Affiliation*

*Address*

*Country*

author2@work

*Author Three*

*Affiliation*

*Address*

*Country*

author3@work