

RcppGO

Peter Kehler*

June 16, 2013

Contents

1	Introduction	1
2	Installation	1
2.1	Requirements	2
2.2	Installation procedure	2
3	Examples	3
3.1	The <code>RcppGO()</code> function	3
3.1.1	A one dimensional optimization problem	4
3.1.2	A multi-dimensional optimization problem	6
3.1.3	Constrained optimization	7
3.2	The <code>RcppGO.Plot()</code> function	7
A	Appendix	10
A.1	The parameters of <code>RcppGO()</code>	10
A.2	The parameters of <code>RcppGO.Plot()</code>	10

1 Introduction

Different kinds of optimization problems require a dedicated algorithm. "[...], optimization algorithms are guided by objective functions. A function is difficult from a mathematical perspective in this context if it is not continuous, not differentiable, or if it has multiple maxima and minima."¹ The aim of the `RcppGO` package is to provide an algorithm to tackle difficult optimization problems as defined before. The algorithm utilizes Newton's laws of gravity and motion and is loosely based on Kaveh and Talatahari [6]. In the interest of brevity the user guide provides only the steps to get started with the package. A detailed article on the algorithm is in preparation. The `RcppGO` package relies on the `Rcpp`² and the `RcppArmadillo`³ packages.

The guide is organized as follows. Section 2 describes how to install the `RcppGO` package. Section 3 presents two examples of application and goes into the differences for uni- and multidimensional optimization problems.

2 Installation

The `RcppGO` package is available on GITHUB. As of today a manual installation process is required. This section describes the steps needed to install the `RcppGO` package after downloading it. For further convention we assume that you saved the package in your download folder.

*Email: peter.kehler.jr@gmail.com

¹Weise [21, p. 56]

²Eddelbuettel and Francois [3]

³Eddelbuettel et al. [4], Sanderson [19]

2.1 Requirements

RcppG0 depends on the R packages Rcpp⁴ and RcppArmadillo⁵. R can be downloaded at the CRAN homepage. The installation of R is documented in R Development Core Team [18].

Package	Version
R	$\geq 2.14.1$
Rcpp	$\geq 0.9.11$
RcppArmadillo	$\geq 0.3.2.0$
RcppDE	$\geq 0.1.0$

Table 1: RcppG0 installation requirements. The RcppDE package is optional and will be needed for performance comparison.

After installing R you can invoke the installation of the other packages via the command in listing 1.

```
1 install.packages(c("Rcpp", "RcppArmadillo", "RcppDE"))
```

Listing 1: Installing required packages within R

2.2 Installation procedure

There are two options to install RcppG0 on your machine. You can either use the **shell** commands provided below or modify and use a prefabricated **shell** script. A prefabricated self-executing⁶ **shell** script can be found in the RcppG0 package. The steps are:

- (a) define Rcpp flags ⁷
- (b) export the defined Rcpp flags
- (c) call the R command to install the RcppG0 package

The following listing shows the commands that have to be executed in the **shell**. First open your **shell** and go to the folder where the RcppG0 package is located, e.g. your download folder.

```
1 cd "~/Downloads/"
```

Listing 2: Open terminal and go to the RcppG0 folder

Following the installation steps outlined above, enter the following commands in the **shell** window. The “#” sign is for comments only.

```
1 # define flags
2 RCPP_CXXFLAGS='Rscript -e 'Rcpp::CxxFlags()''
3 RCPP_LIBS='Rscript -e 'Rcpp::LdFlags()''
4 RCPP_ARMADILLO='Rscript -e 'RcppArmadillo::CxxFlags()''
5
6 # export flags
7 export PKG_CPPFLAGS="${RCPP_ARMADILLO} ${RCPP_CXXFLAGS}"
8 export PKG_LIBS="-larmadillo -llapack ${RCPP_LIBS}"
9
10 ## call the R install command
11 R CMD INSTALL RcppG0*
```

Listing 3: Commands for the installation via the **shell** command line

⁴Eddelbuettel and Francois [3]

⁵Eddelbuettel et al. [4], Sanderson [19]

⁶In order to execute the script the user may need to change the mode of the script. This can be done via a **shell** command provided in the script.

⁷See the R Development Core Team [16, chapter 5] manual for further information.

If the procedure worked correct, the output on your console should look like this:

```
1 ** R
2 ** preparing package for lazy loading
3 ** help
4 *** installing help indices
5 ** building package indices ...
6 ** testing if installed package can be loaded
7 *** arch - i386
8 *** arch - x86_64
9
10 * DONE (RcppG0)
```

Listing 4: Terminal output

After installing the package it can be loaded into your R session.

```
1 library(RcppG0)
```

Listing 5: Loading packages into R

Loading the RcppG0 package loads also the packages RcppG0 depends on. After loading the library into R the help page of the RcppG0 package is available. Type the following command in R to open it:

```
1 help("RcppG0")
```

Listing 6: Opening help page

The help page gives a short description of the package, its functions, their parameters and two introductory examples.

In the future the RcppG0 package will be available via CRAN. This will simplify the installation process on the user side to:

```
1 install.packages{"RcppG0"}
```

Listing 7: Installation via CRAN

3 Examples

The RcppG0 package contains two functions. RcppG0() for calling the optimization routine and RcppG0.Plot() for various plots of two dimensional functions. In this section introductory examples of the RcppG0() function will be given.

Remark 3.1. *The following conventions are used in this guide.*

1. *The examples assume that the objective function is to be minimized.*
2. *The capitalized letters in the R code indicate a matrix notation instead of a vector notation.*

3.1 The RcppG0() function

The two optimization problems included in the help pages utilize variants of the ALUFFI-PENTINY⁸ function as objective functions. It is important for the user to understand, that one and multi-dimensional optimization problems are treated differently in RcppG0. They differ in their definition. Before two detailed examples are given, the general steps of how to handle optimization problems with RcppG0 are defined:

⁸The ALUFFI-PENTINY function is a standard function used to benchmark optimization algorithms. See Yang [23], Yang [22], Molga and Smutnicki [12] for further details.

- (a) Define the objective function (optional: add constraints)⁹,
- (b) define search space, and the `RcppG0()` specific parameters¹⁰,
- (c) store the calculations in an R object,
- (d) and print the results.

3.1.1 A one dimensional optimization problem

The first example in the help pages contains a one dimensional ALUFFI-PENTINY objective function. The objective function is given by:

$$f(x) = \frac{1}{4}x^4 - \frac{1}{2}x^2 + \frac{1}{10}x + \frac{1}{2}x^2 \quad (1)$$

The minimum is located at approximately $x = -0.46415$ with $f(x) = -0.03481$. As outlined above the objective function has to be defined in R.

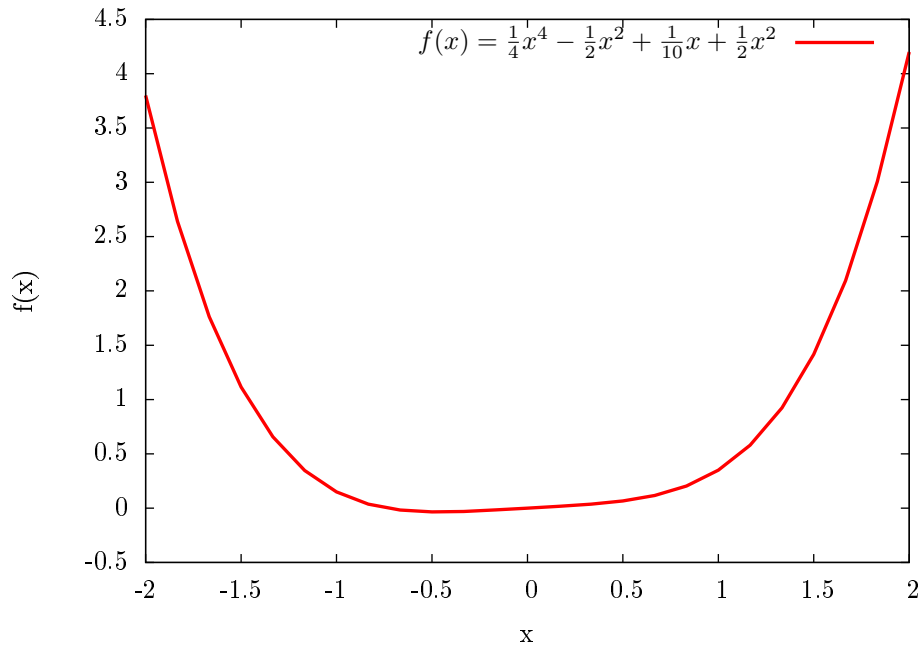


Figure 1: The ALUFFI-PENTINY function

```

1 # Defining f(x) = 1/4 x^4 - 1/2 x^2 + 1/10 x + 1/2 x^2 in R
2
3 AluffiPentiny01 <- function(X)
4 {
5   1/4*X^4 - 1/2*X^2 + 1/10*X + 1/2*X^2
6 }

```

Listing 8: Defining objective function (1) in R

Following the steps outlined before, the search space and the `RcppG0()` function specific parameters have to be defined.

⁹See section 3.1.3.

¹⁰See A.1

```

1 Example01_Output <- RcpgG0(           # store calculations in an R object
2 ObjectiveFunction=AluffiPentiny01,    # passing the objective function
3 Args=1,                              # define the number of arguments
4 Lower = -10,                         # define lower limit of search space
5 Upper = 10                           # define upper limit of search space
6 )

```

Listing 9: defining the parameters of RcpgG0()

See section A.1 for a detailed description on all parameters of RcpgG0. Before the results are accessed, the structure of Example01_Output is explained. Typing `str(Example01_Output)` into the R console reveals the composition of Example01_Output.

```

1 > str(Example01_Output)               # structure of the results
2 List of 12
3 $ GravityParticles : num [1:20, 1:4, 1:200] -0.2349 -0.2246 0.0854 1.2793 -1.5062 ...
4 .. attr(*, "dimnames")=List of 3
5 .. ..$ : chr [1:20] "1" "2" "3" "4" ...
6 .. ..$ : chr [1:4] "x1" "fn_x" "v_x1" "F_x1"
7 .. ..$ : NULL
8 $ ObjectiveFunction:function (X)
9 .. attr(*, "srcref")=Class 'srcref' atomic [1:8] 1 20 4 1 20 1 1 4
10 .. .. attr(*, "srcfile")=Classes 'srcfilecopy', 'srcfile' <environment: 0x20f7ae0>
11 $ GMemory          : num [1:20, 1:2] -0.464 -0.464 -0.464 -0.464 -0.464 ...
12 .. attr(*, "dimnames")=List of 2
13 .. ..$ : chr [1:20] "1" "2" "3" "4" ...
14 .. ..$ : chr [1:2] "x1" "fn_x"
15 $ Iterations       : num 200
16 $ Args             : int 1
17 $ n                : int 20
18 $ g                : int 20
19 $ Lower            : num -10
20 $ Upper            : num 10
21 $ Scale            : num 0.1
22 $ User             : logi FALSE
23 $ Maximize         : logi FALSE

```

Listing 10: Understanding the results

Line 2 of listing 10 shows that `str(Example01_Output)` is a list of 12 objects. The results of the optimization process are stored in GMemory. The acces of single objects is done via the listname followed by a \$ sign and the list object, as shown in the following listing.

```

1 > Example01_Output$GMemory           # print the results
2      x1      fn_x
3 1 -0.4641558 -0.03481192
4 2 -0.4641725 -0.03481192
5 3 -0.4641759 -0.03481192
6 4 -0.4641796 -0.03481192
7 5 -0.4641825 -0.03481192
8 6 -0.4641857 -0.03481192
9 7 -0.4641860 -0.03481192
10 8 -0.4641264 -0.03481192
11 9 -0.4641917 -0.03481192
12 10 -0.4641940 -0.03481192

```

Listing 11: Accessing the results

The stochastic results match the theoretical results.

3.1.2 A multi-dimensional optimization problem

In order to enable the user to define complex functions with an arbitrary amount of variables, the `RcppG0` objective function has to be written in matrix notation.¹¹ Here is an example for the two dimensional `ALUFFIPENTINY` function.

```

1 # min at -0.352386, X in [-10,10]^2
2 AluffiPentiny02 <- function(X)
3 {
4   1/4*X[,1]^4 - 1/2*X[,1]^2 + 1/10*X[,1] + 1/2*X[,2]^2
5 }

```

Listing 12: Defining equation (1) in R using matrix notation

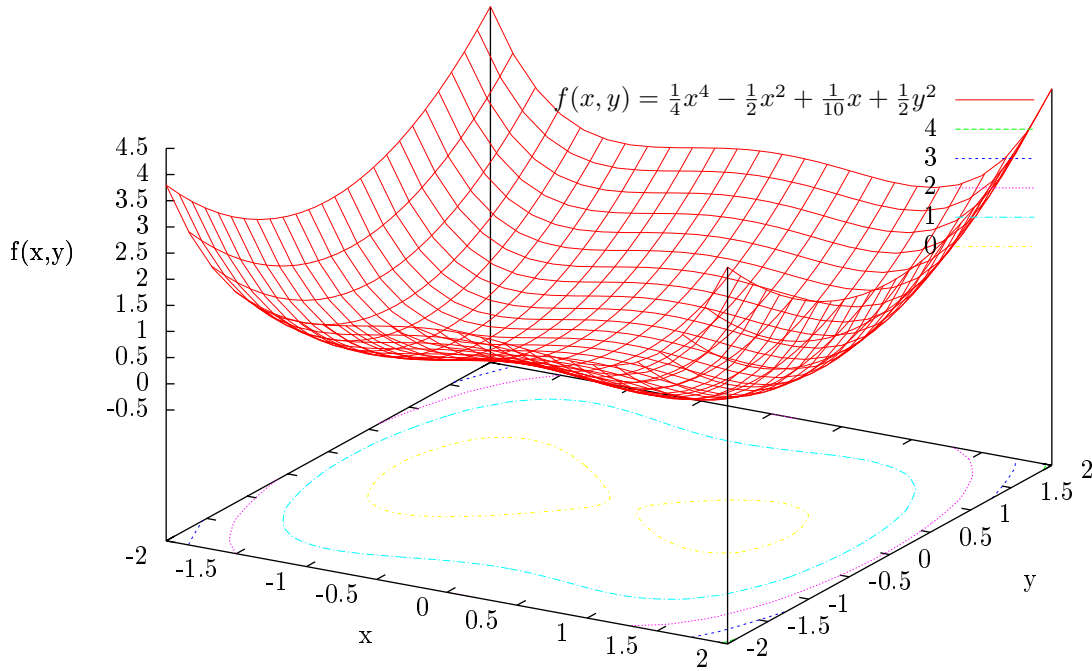


Figure 2: The two dimensional `ALUFFIPENTINY` function.

Assuming the user wants to compute an approximate of the best solutions in the lower bounds of $\mathbf{x}_{lower} = \begin{pmatrix} -10 \\ -10 \end{pmatrix}$ and upper bounds $\mathbf{x}_{upper} = \begin{pmatrix} 10 \\ 10 \end{pmatrix}$, the optimization process can be initialized as follows:

```

1 > Example02 <- RcppG0(ObjectiveFunction=AluffiPentiny, Args=2, Lower = -10, Upper = 10)

```

Listing 13: Initializing the optimization process

The output of the optimization process is assigned to the variable `Example02`. In its current form the `RcppG0` contains additional information needed e.g. for the `RcppG0.Plot` function. Typing `Example02` would result in a long chain of output.¹² To access the results only the user has to access an element of the list, called `GMemory` in R, as shown below:

¹¹The matrix notation `X[1,2,]` means: Access the the element in row 1 in coloumn 2. Therefore `X[,2]` means: Access all elements in coloumn 2.

¹²The structure of `Example02` is a list. You can see that by typing `str(Example02)` in the R console.

```

1 > Example02$GMemory
2       x1       x2       fn_x
3 1 -1.045695 -0.0008089336 -0.3523846
4 2 -1.043545  0.0085946639 -0.3523379
5 3 -1.049650 -0.0112856804 -0.3523123
6 4 -1.036312 -0.0061996451 -0.3522451
7 5 -1.050161  0.0163825537 -0.3522380
8 6 -1.059847 -0.0025767241 -0.3521822
9 7 -1.033795  0.0109659926 -0.3521384
10 8 -1.031220 -0.0060378656 -0.3520984
11 9 -1.072199 -0.0038773126 -0.3516166
12 10 -1.062366 -0.0334229455 -0.3515422

```

Listing 14: R output

The output rows show the top ten solutions generated during the optimization process. The first two columns represent the coordinates where the solutions were found and the third column exhibits the corresponding function values.

3.1.3 Constrained optimization

(TODO: AN APPROACH FOR CONSTRAINT OPTIMIZATION WILL BE ADDED IN THE FUTURE.)

3.2 The RcppG0.Plot() function

The RcppG0.Plot function is a wrapper around a few `lattice` and R functions and enables the user to visualize the structure of two dimensional optimization problems. Following the example from section 3.1.2 listing 15 shows how to call the plot function.¹³

```

1 RcppG0.Plot(RcppG0.Data=Example02)

```

Listing 15: RcppG0.Plot function

Figure 3 shows the result in R. The image consists of two panels. The left one exhibits a relief-like view of the objective function and the right one shows a contourplot. In both plots the function values are coloured in topographical colours.

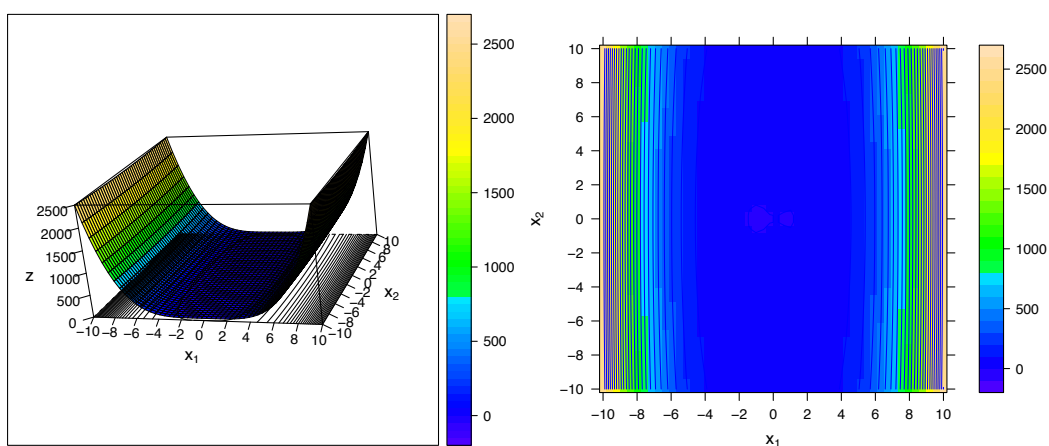


Figure 3: The RcppG0.Plot function with `Particle_Sim=FALSE`

Invoking the RcppG0.Plot function with `Particle_Sim=TRUE` visualizes the search process in an particle movement animation. The graph is updated in intervalls controlled via the `Delayed` option. If

¹³Further details of the plot function are presented in section A.2.

Physics=TRUE, the resulting force on any particle is visualized, as well as the current velocity and the position of the particles in $t + 1$.¹⁴

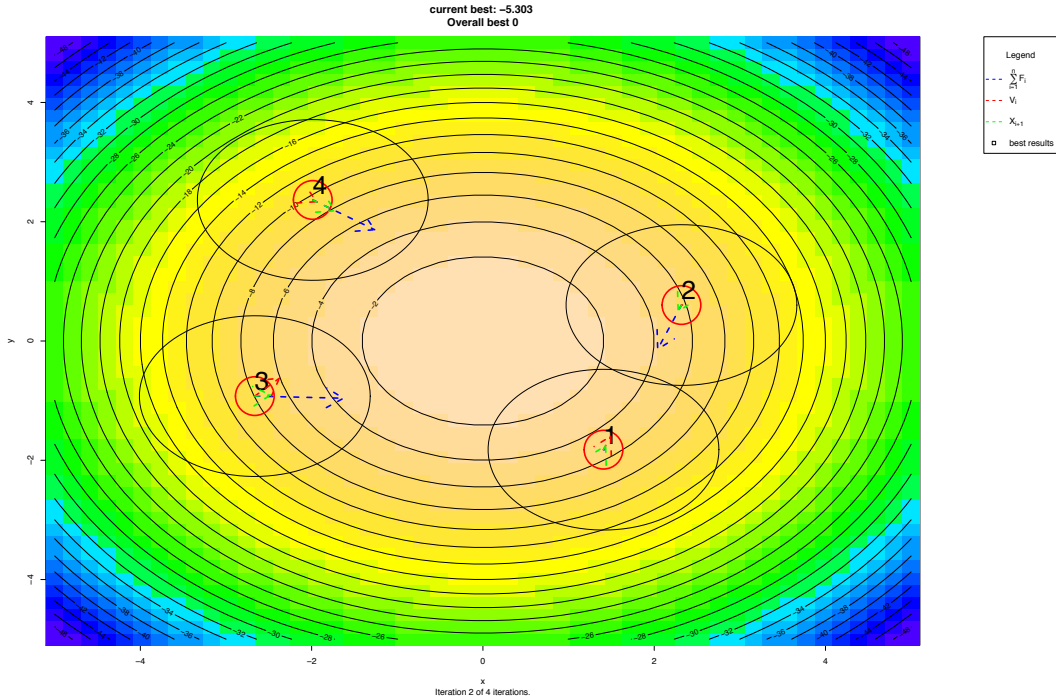


Figure 4: The RcppG0.Plot function with Particle_Sim=TRUE of $f(x, y) = x^2 + y^2$.

References

- [1] Dirk Eddebuetel and Romain Francois. Extending Rcpp. 2011.
- [2] Dirk Eddebuetel. From DEoptim to RcppDE: A case study in porting from C to C++ using Rcpp and RcppArmadillo. 2011.
- [3] Dirk Eddebuetel and Romain Francois. Writing a package that uses Rcpp. 2011.
- [4] Dirk Eddebuetel, Romain Francois, and Douglas Bates. RcppArmadillo: Rcpp integration for Armadillo templated linear algebra library. 2010. URL <http://cran.r-project.org/package=RcppArmadillo>.
- [5] A. Kaveh and S. Talatahari. A Charged System Search With A Fly To Boundary Method For Discrete Optimum Design Of Truss Structures. *Asian Journal Of Civil Engineering (Building And Housing)*, 11(3):277–293, 2010.
- [6] A Kaveh and S Talatahari. A Novel Heuristic Optimization Method: Charged System Search. *Acta Mechanica*, 213(3-4):267–289, 2010. ISSN 0001-5970. doi: 10.1007/s00707-009-0270-4.
- [7] Ali Kaveh and Siamak Talatahari. An Enhanced Charged System Search For Configuration Optimization Using The Concept Of Fields Of Forces. *Structural and Multidisciplinary Optimization*, pages 1–13, 2010.
- [8] Ali Kaveh and Siamak Talatahari. Geometry And Topology Optimization Of Geodesic Domes Using Charged System Search. *Structural and Multidisciplinary Optimization*, pages 1–15, 2010.
- [9] Ali Kaveh and Siamak Talatahari. Optimal Design Of Skeletal Structures Via The Charged System Search Algorithm. *Structural and Multidisciplinary Optimization*, 41(6):893–911, 2010.
- [10] Ali Kaveh and Siamak Talatahari. A general model for meta-heuristic algorithms using the concept of fields of forces. *Acta Mechanica*, 221:99–118, 2011.

¹⁴See the legend of 4.

- [11] Ali Kaveh, Siamak Talatahari, and R. Sheikholeslami. An efficient charged system search using chaos for global optimization problems. *International Journal of Optimization in Civil Engineering*, 2:305–325, 2011.
- [12] Marcin Molga and Czesław Smutnicki. Test functions for optimization needs. 2005.
- [13] K.M. Mullen, D. Ardia, D.L. Gil, D. Windover, and J. Cline. DEoptim: An R Package for Global Optimization by Differential Evolution. *Journal of Statistical Software*, 40(6):1–26, 2011.
- [14] Magnus Erik Hvass Pedersen. *Tuning & Simplifying Heuristical Optimization*. PhD thesis, University of Southampton Computational Engineering and Design Group School of Engineering Sciences, 2010.
- [15] R Development Core Team. *R: A Language And Environment For Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria, 2011. URL <http://www.r-project.org>.
- [16] R Development Core Team. *Writing R Extensions*, 2012.
- [17] R Development Core Team. *The R language definition*, 2012.
- [18] R Development Core Team. *R Installation and Administration*, 2012.
- [19] Conrad Sanderson. Armadillo: An open source C++ Algebra Library for Fast Prototyping and Computationally Intensive Experiments. Technical report, NICTA, 2010. URL <http://arma.sourceforge.net>.
- [20] P. A. Tipler and G. Mosca. *Physics for scientists and engineers*, volume 1. Macmillan, 2008.
- [21] Thomas Weise. *Global Optimization Algorithms - Theory and Application*. 2009.
- [22] Xin-She Yang. *Engineering Optimization: An Introduction with Metaheuristic Applications*. John Wiley & Sons, 2010.
- [23] Xin-She Yang. Test problems in optimization. *Department of Engineering, University of Cambridge, Cambridge CB2 1PZ, UK*, 2010.

A Appendix

This section serves as a brief overview of the `RcppG0` functions. For further details read the upcoming article corresponding to the package.

A.1 The parameters of `RcppG0()`

The `RcppG0` function is the core of the `RcppG0` package. At its heart lies the call to the optimization algorithm written in C++. The `RcppG0` function has ten parameters as of today.

- **ObjectiveFunction**: The objective function to be optimized. Be aware of the matrix notation.
- **Args**: Defines the number of objective function arguments.
- **Lower, Upper**: Vectors specifying the lower and upper bounds of the optimization routine.
- **n**: The number of particles to be used in the optimization process. The default is 20.
- **g**: The number of solutions to be saved. **g** should be less or equal to **n**. The default value is 20.
- **Iterations**: Specifying the number of iterations after the algorithm terminates. Default is 200.
- **Scale**: A parameter for definig the attraction radius of the search particles. Default is 0.1.
- **User**: If the user wants to controll the **Scale** parameter manually, set **User=TRUE**. Default is **FALSE**.
- **Maximize**: Control parameter for maximizing (**Maximize=TRUE**) or minimizing (**Maximize=FALSE**) the objective function.

As mentioned before the `RcppG0`-function returns a list. **(TODO: INSERT REFERENCE)**

A.2 The parameters of `RcppG0.Plot()`

The `RcppG0.Plot` function is an attempt to visualize the optimization process. In its current state only two dimensional problems can be visualized. Support for one dimensional problems might be added in the future.

As mentioned before the `RcppG0` function returns a list. The results of the `RcppG0` function are sufficient for the plot function.

- **RcppG0.Data**: Requires the output from the `RcppG0` function.
- **Delayed**: Controls the delay of the moving particles in seconds. Default value is 0.3.
- **Particle_Sim**: If **FALSE** a static image with a contourplot and a 3D plot of the objective function will be printed to the screen. If **TRUE** a contourplot with the animated movement of the particles will be displayed.
- **Physics**: **Physics=TRUE** turns on the the resultant force on a particle (blue), the resultant velocity (red) and the position in $t + 1$ (green).
- **...**: The ... parameter allows the user to put parameters through to a user defined function.