



## Numerical Optimization in R: Beyond `optim`

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### Abstract

Numerical optimization is often an essential aspect of mathematical analysis in science, technology and other areas. The function `optim()` provides basic optimization capabilities and is among the most widely used functions in R. Additionally, there are various packages and functions for solving various types of optimization problem (the optimization task view on Comprehensive R Archive Network provides a comprehensive list of available options for solving optimization problems in R). In this special volume, four papers are presented which discuss some of the areas in numerical optimization where significant developments have been made recently to enhance the capabilities in R. This introduction provides a brief overview of the volume.

*Keywords:* optimization algorithms, global optimization, convex programming, spectral gradient, constraints.

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Numerical optimization is often an essential aspect of mathematical analysis in science, technology and other areas. R (R Core Team 2014) provides various packages and functions for conducting optimization. The function `stats::optim`, or, simply, `optim`, provides basic optimization capabilities and may easily be among the most widely used functions in R. By *basic optimization* is meant the optimization of a smooth objective function without any constraints, or at most, with box constraints on the parameters.

In this special volume, four papers are presented which discuss some of the areas in numerical optimization where significant developments have been made recently to enhance the capabilities in R.

- A report on the ongoing work by Nash (2014) discusses best-practice methods for optimization to replace the default algorithms available in `optim` which were developed more than 40 years ago. For example, the package `optimx` (Nash and Varadhan 2011) contains several of such best-practice algorithms.
- Birgin, Martinez, and Raydan (2014) provide a review of a class of gradient-based methods, spectral projected gradient method, for solving high-dimensional, constrained

optimization problems. This method has been implemented in a function called `spg` in the R package **BB** (Varadhan and Gilbert 2009).

- A trust-region based algorithm for the unconstrained optimization of a smooth objective function, with sparse Hessians, is proposed by Braun (2014). This is mainly useful for finding the mode of log-posterior density in Bayesian models with a large number of parameters, where the Hessian is sparse.
- Koenker and Mizera (2014) provide an overview of techniques for solving convex optimization problems in R by , with a particular focus on problems arising in computational statistics. The paper highlights a solution approach that leverages a powerful, commercially-available, convex programming solver, **MOSEK** (MOSEK ApS, Denmark 2011), which is linked to R via the package **Rmosek**.
- Mullen (2014) presents a comprehensive review and evaluation of numerous algorithms for finding the global optimum of a smooth function. She compares 18 algorithms for global optimization on a suite of test functions which are available in a new R called **globalOptTests**.

This special volume is by no means a comprehensive survey of all the recent developments. Our main goal is to increase the awareness of the optimization user in R to some of the relatively recent and useful options available for solving optimization problems, extending beyond `optim`. We encourage the reader to take a look at the CRAN (Comprehensive R Archive Network) task view on optimization (Theussl 2014) for a comprehensive list of available packages for solving optimization problems in R.

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## References

- Birgin EG, Martinez JM, Raydan M (2014). “Spectral Projected Gradient Methods: Review and Perspectives.” *Journal of Statistical Software*, **60**(3), 1–21. URL <http://www.jstatsoft.org/v60/i03/>.
- Braun M (2014). “**trustOptim**: An R Package for Trust Region Optimization with Sparse Hessians.” *Journal of Statistical Software*, **60**(4), 1–16. URL <http://www.jstatsoft.org/v60/i04/>.
- Koenker R, Mizera I (2014). “Convex Optimization in R.” *Journal of Statistical Software*, **60**(5), 1–23. URL <http://www.jstatsoft.org/v60/i05/>.
- MOSEK** ApS, Denmark (2011). *The MOSEK Optimization Tools Manual*. Version 6.0, URL <http://www.mosek.com/>.

- Mullen K (2014). “Continuous Global Optimization in R.” *Journal of Statistical Software*, **60**(6), 1–45. URL <http://www.jstatsoft.org/v60/i06/>.
- Nash JC (2014). “On Best Practice Optimization Methods in R.” *Journal of Statistical Software*, **60**(2), 1–14. URL <http://www.jstatsoft.org/v60/i02/>.
- Nash JC, Varadhan R (2011). “Unifying Optimization Algorithms to Aid Software System Users: **optimx** for R.” *Journal of Statistical Software*, **43**(9), 1–14. URL <http://www.jstatsoft.org/v43/i09/>.
- R Core Team (2014). *R: A Language and Environment for Statistical Computing*. R Foundation for Statistical Computing, Vienna, Austria. URL <http://www.R-project.org/>.
- Theussl S (2014). “CRAN Task View: Optimization and Mathematical Programming.” Version 2014-08-08, URL <http://CRAN.R-project.org/view=Optimization>.
- Varadhan R, Gilbert P (2009). “**BB**: An R Package for Solving a Large System of Nonlinear Equations and for Optimizing a High-Dimensional Nonlinear Objective Function.” *Journal of Statistical Software*, **32**(4), 1–26. URL <http://www.jstatsoft.org/v32/i04/>.

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