

Unifying optimization algorithms in R for smooth, nonlinear problems

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The `optim()` function in the R 'stats' collection provides a powerful yet clean and easy-to-use mechanism for users to launch optimization tasks. Over the years, however, other packages have been introduced in order to provide for special or supposedly more-efficient capabilities. We present some work to unify these tools and to help the user make sensible choices, but aim to retain the essential tidiness of the interface. We welcome commentary and assistance from the R and optimization communities to further these efforts.

Our objectives are:

1. To unify optimization tools in R for solving smooth, nonlinear, box-constrained optimization problems.
2. To provide “guidance” to users for choosing the appropriate algorithm, automatically setting up the appropriate function call essentially in the same style as `optim()`.
3. To update/extend algorithms in `optim()`

One motivation for this work is that the early tools (Nelder-Mead, CG, BFGS) were chosen and adapted by one of us (Nash, 1979) for use on very limited systems three decades ago. They are still very usable and useful tools, but we believe that users need to be led to choices better suited to their problems given the evolution of both statistical problems and optimization techniques.

Further, many statistical workers are not familiar with the difficulties that attend optimization, so we also wish to provide better defaults and better guidance on the use of a new `optim()`. We want a new method, really a wrapper for other methods, that we call “GUIDED” that will assist the user in creating the `optim()` syntax. In this we take inspiration from the Decision Tree for Optimization Software (Mittelman, 2008). Further, we believe some new developments in optimization such as Powell's (2007) BOBYQA are likely better candidates for the default tool than Nelder-Mead.

The GUIDED selection also promotes a unification of optimization methods within R. The `optim()` function supports only a small subset of the available tools from different packages. We would like to provide hooks to allow different optimization approaches to be called using the `optim()` structure. Related questions can be posed about cleanly linking `optim()` to related tools such as `nls()`, both in the computational structures and in the documentation.

References

Nash J C (1979) Compact numerical methods for computers: linear algebra and function minimisation, Bristol: Adam Hilger.

Mittelman H (2008) Decision Tree for Optimization Software,
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Powell M J D (2007) *Developments of NEWUOA for minimization without derivatives*,
www.damtp.cam.ac.uk/user/na/NA_papers/NA2007_05.pdf. (Note: The BOBYQA software is described, but was not released until January 2009 pending selection of some options to be set as defaults.)