

lbfgsb3x: Using the 2011 version of L-BFGSB

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Abstract

In 2011 the authors of the L-BFGSB program published a correction and update to their 1995 code. The latter is the basis of the L-BFGS-B method of the `optim()` function in base-R. The package `lbfgsb3x` is a merging of CRAN packages `lbfgsb3` and `lbfgsb3c`. This vignette gives a brief explanation of the offerings of this package.

Provenance of the R `optim::L-BFGS-B` and related solvers

The base-R code `lbfgsb.c` (at writing in R-3.5.2/src/appl/) is commented:

```
/* l-bfgs-b.f -- translated by f2c (version 19991025).
```

```
From ?optim:
```

```
The code for method "L-BFGS-B" is based on Fortran code by Zhu,  
Byrd, Lu-Chen and Nocedal obtained from Netlib (file 'opt/lbfgs_bcm.shar')
```

```
The Fortran files contained no copyright information.
```

```
Byrd, R. H., Lu, P., Nocedal, J. and Zhu, C. (1995) A limited  
memory algorithm for bound constrained optimization.  
\emph{SIAM J. Scientific Computing}, \bold{16}, 1190--1208.
```

```
*/
```

The paper R. H. Byrd, Lu, Nocedal, and Zhu (1995a) builds on Lu et al. (1994). There have been a number of other workers who have followed-up on this work, but **R** code and packages seem to have largely stayed with codes derived from these original papers. Though the date of the paper is 1995, the ideas it embodies were around for a decade and a half at least, in particular in Nocedal80 and LiuN89. The definitive Fortran code was published as Zhu et al. (1997). This is available as `toms/778.zip` on www.netlib.org. A side-by-side comparison of the main subroutines in the two downloads from Netlib unfortunately shows a lot of differences. I have not tried to determine if these affect performance or are simply cosmetic.

More seriously perhaps, there were some deficiencies in the code(s), and in 2011 Nocedal's team published a Fortran code with some corrections (Morales and Nocedal (2011)). Since the **R** code predates this, I prepared package `lbfgsb3` (Nash et al. (2015)) to wrap the Fortran code. However, I did not discover any test cases where the `optim::L-BFGS-B` and `lbfgsb3` were different, though I confess to only running some limited tests. There are, in fact, more in this vignette.

In 2016, I was at a Fields Institute optimization conference in Toronto for the 70th birthday of Andy Conn. By sheer serendipity, Nocedal did not attend the conference, but sat down next to me at the conference dinner. When I asked him about the key changes, he said that the most important one was to fix the computation of the machine precision, which was not always correct in the 1995 code. Since **R** gets this number as `.Machine$double.eps`, the offending code is irrelevant.

Within Morales and Nocedal (2011), there is also reported an improvement in the subspace minimization that is applied in cases of bounds constraints. Since few of the tests I have applied impose such constraints, it is reasonable that I will not have observed performance differences between the base-R `optim` code and my `lbfgsb3` package. More appropriate tests are welcome, and on my agenda.

Besides the ACM TOMS code, there are two related codes from the Northwestern team on NETLIB: http://netlib.org/opt/lbfgs_um.shar is for unconstrained minimization, while http://netlib.org/opt/lbfgs_bcm.shar handles bounds constrained problems. To these are attached references Liu and Nocedal (1989) and R. H. Byrd, Lu, Nocedal, and Zhu (1995b) respectively, most likely reflecting the effort required to implement the constraints.

The unconstrained code has been converted to **C** under the leadership of Naoaki Okazaki (see <http://www.chokkan.org/software/liblbfgs/>, or the fork at <https://github.com/MIRTK/LBFGS>). This has been wrapped for **R** as Coppola, Stewart, and Okazaki (2014) as the **lbfgs** package. This can be called from `optimx::optimr()`.

Using Rcpp (see Eddelbuettel and François (2011)) and the Fortran code in package **lbfgs3**, Matthew Fidler developed package **lbfgsb3c** (Fidler et al. (2018)). As this provides a more standard call and return than **lbfgsb3** Fidler and I are unified the two packages as **lbfgsb3x**.

Functions in package **lbfgsb3x**

There are four optimizer functions in the package:

- **lbfgsb3**, which uses a **.Fortran** call of the compiled 2011 Fortran code. The object returned by this routine is NOT equivalent to the object returned by base-R `optim()` or by `optimx::optimr()`. Instead, it includes a structure **info** which contains the detailed diagnostic information of the Fortran code. For most users, this is not of interest, and I only recommend use of this function for those needing to examine how the optimization has been carried out.
- **lbfgsb3f()** wraps **lbfgsb3()** to produce a returned object of the same form as `optim()`.
- **lbfgsb3c()** uses Rcpp (Eddelbuettel (2013), Eddelbuettel and François (2011), Eddelbuettel and Balamuta (2017)) to streamline the call to the underlying Fortran.
- **lbfgsb3x()** is an alias of **lbfgsb3c()**

We recommend using the **lbfgsb3c()** call for most uses.

References

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