
Lianjun Jiang
**A preconditioned L-BFGS algorithm with application to
protein structure prediction**

1475 Folsom st
apt 171
Boulder
CO 80302
lianjunj@gmail.com
Richard Byrd
Elizabeth Eskow
Robert B. Schnabel

The limited-memory BFGS method has been widely used in large scale unconstrained optimization problems, including protein structure prediction. A major weakness of the L-BFGS method is that it may converge very slowly for ill-conditioned problems. We propose a preconditioned L-BFGS method, where we form the preconditioner from parts of the partially separable objective function. We report results of experiments in the context of the protein structure prediction problem for four different proteins, using a protein energy model as the objective function and multiple initial configurations for each protein. The results show speed-ups with factors between 3 and 10 in terms of function evaluations and with factors between 2 and 7 in terms of CPU time. The difference between CPU time and function evaluation speed-up is due to the extra overhead of calculating and applying the preconditioner. We also compare our results to a method from the other competitive class of large-scale methods, preconditioned truncated Newton method (TNPack). The limited results indicate that the preconditioned L-BFGS method may be more efficient.

We also tried this approach in a more general context, using limited memory with an incomplete Cholesky factorization of the Hessian as a preconditioner. We compared the performance with the truncated Newton algorithm TRON, which uses a similar preconditioner. Tested on a subset of the CUTER test problems, our results show that, using this preconditioner, the preconditioned LBFGS method is competitive with TRON and much better than the LBFGS algorithm without preconditioner.