Direct Search Methods for Optimization

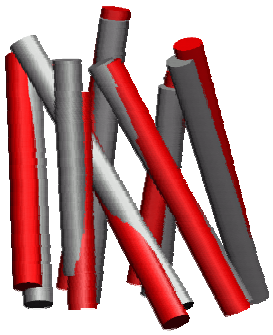
Direct search methods are best known as unconstrained optimization techniques that do not explicitly use derivatives. These methods are extremely useful in simulation-based optimization, where derivative information is often unavailable.

In collaboration with Virginia Torczon at the College of William and Mary, we previously developed the Asynchronous Parallel Pattern Search (APPS) algorithm [1] and accompanying APPSPACK software, available via the GNU L-GPL license.

Continuing the work with Torczon, we have since analyzed the convergence behavior of the APPS algorithm. If the function to be optimized is continuously differentiable, then APPS is guaranteed to converge to a stationary point. See Kolda and Torczon [2,3] for more details.

The most recent endeavor into the theoretical side of direct search methods is a review paper [4] with Torczon and R. Michael Lewis, also at the College of William and Mary. We present a framework called "Generating Set Search" (GSS) that captures the key features in pattern search and closely related methods. We present a unified analysis of GSS that illuminates why these methods work.

Genetha Gray has spearheaded collaboration with Malin Young and Ken Sale in the Biosystems Research Department at Sandia to consider the problem of transmembrane protein structure prediction. APPSPACK was able to solve the problem both more quickly and more accurately than the simulated annealing optimization approach they had been using previously. In the figure that follows, we show an example problem with a protein of known structure denoted in gray. The prediction by APPSPACK is shown in red and corresponds to an RMSD of 3.4, as good as can be expected given the noise in the data.



We have several ongoing internal collaborations in other applications areas such as electrical circuit simulation and forging design and analysis. Externally, our most recent collaboration is with David Keyes of Columbia University on parameter fitting for wildfire simulations.

[1] P. D. Hough, T. G. Kolda, and V. J. Torczon, *Asynchronous Parallel Pattern Search for Nonlinear Optimization*, SIAM J. Scientific Computing, 23(1):134-156, June 2001.

[2] Tamara G. Kolda and Virginia Torczon, *On the convergence of asynchronous parallel pattern search*, SIAM J. Optimization, to appear.

[3] Tamara G. Kolda and Virginia Torczon. *Understanding asynchronous parallel pattern search*. High Performance Algorithms and Software for Nonlinear Optimization, Kluwer Academic Publishers, to appear.

[4] Tamara G. Kolda, R. Michael Lewis, and Virginia Torzon, *Direct Search Methods: A Selective Review*, SIAM Review, to appear September 2003.

Contacts

Tamara Kolda (PI)
Sandia Natl. Labs
Livermore, CA
925-294-4769
tgkolda@sandia.gov

Genetha Gray
Sandia Natl. Labs
Livermore, CA
925-294-4957
gagray@sandia.gov

Web Page

http://software.sandia.gov/appspack