Computational Differentiation in Global Optimization Software

This talk will present:

1. The general problem framework in optimization software.
2. An example of effectiveness of computational differentiation in optimization packages.
3. Particular importance of computational differentiation verified global optimization.
4. A simple example of use of our package.
5. Outline of the present structure.
6. Developments in the near future.
7. Relationships with other work presented here.

The General Problem Framework

Traditional Optimization Packages

- Traditional non-verified global optimization algorithms require *objective function*, *gradient*, and *Hessian matrix.*
- Supplying these without computational differentiation uas been done with *user-supplied derivatives*, *finite-difference approximations*, or *symbolic manipulation packages.*

Traditional Optimization

Disadvantages without Computational Differentiation

User-supplied derivatives can take excessive amounts of labor to get right.

Finite-difference approximations can be both numerically inaccurate and take more computer resources than necessary.

Symbolic manipulation packages are subject to *expression swell* that makes the results impractical to use.

Although only order-2 derivatives are used (in contrast to other problems addressed here), complicated functions and many variables make the above disadvantages real.

Computational Differentiation in Traditional Optimization

A Successful Example

- Computational differentiation can numerically more accurate, in addition to being more labor and computation efficient.
- An example is *Network Enabled Optimization System* (NEOS) server at `www.mcs.anl.gov/otc/Server/`
- Users need only submit subroutines in Fortran or C, and the package uses the computational differentiators ADIFOR or ADOLC to compute derivatives.
- The system runs the solver, and the answer to the problem is sent back through the WWW.