Comparison of Three Descent Methods for TRUST

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http://www.csm.ornl.gov/Internships/abstracts/ChristopherRandall.pdf

Introduction

Nonlinear global optimization problems occur in every field of scientific, technologic, economic, or social interests. The problem consists of finding the global minimum of a function depending on many variables which is typically multi-modal, i.e., it possesses many local minima. Generally, the number of local minima increases exponentially with the problem's dimensionality. The algorithm known as TRUST (Terminal Repeller Unconstrained Subenergy Tunneling) is currently one of the fastest available methods for finding global minima within complex functional landscapes. This poster contains a summary of the research done to compare three different descent methods to be eventually included in TRUST. These methods are: (i) gradient; (ii) conjugate gradient; and (iii) a new descent method called "fractional power adaptive switching gradient descent" (FPASGD). **Assessing the best method is important since even a small gain in local minimization performance may result in an exponential gain in the global optimization problem.**

Global Optimization Challenges

- Typical stopping criterion does not discriminate between global and local minima
- Local minimum solutions are trapped
- Computational speed is slow (high cost)

Innovative Solutions

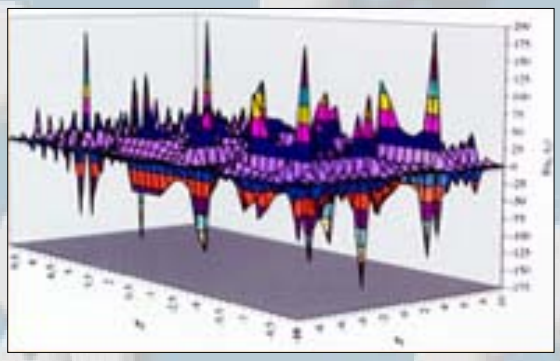
- Subenergy Tunneling
- Terminal Repellers
- FPASGD

Research Objectives

- **Develop** code to compare descent speeds of current local minimization methods to new method based on FPASGD for TRUST
- **Program** code in Visual Fortran 95
- **Test** new algorithm on benchmark functions

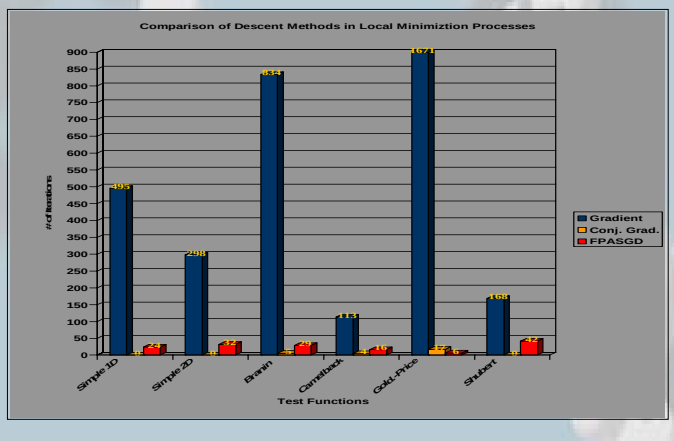
Applications

- Lennard-Jones atomic clusters for DOE-sponsored materials science research
- More accurate characterization of petroleum reservoirs thru seismic exploration for oil industry



Shubert Function: Example of two-dimensional function with multiple local minima

Results



Descent Methods

- **Gradient** - Explicitly uses derivative info to locate minima
- **Conjugate Gradient** - Modifies gradient descent by requiring that successive search directions be mutually conjugate
- FPASGD - Enhances gradient descent by using fractional exponent in the first derivative term

Conclusions

- Successful development of comparison algorithm framework
- FPASGD performs better than gradient method
- Conjugate gradient method applied to a few test functions; complete assessment of comparison is in progress

Potential Future Research

- Complete assessment of descent method comparison
- Addition of a library of multi-dimensional test functions to TRUST

The Research Alliance in Math and Science program is sponsored by the Mathematical, Information, and Computational Sciences Division, Office of Advanced Scientific Computing Research, U.S. Department of Energy. The work was performed at the Oak Ridge National Laboratory, which is managed by UT-Battelle, LLC under Contract No. De-AC05-00OR22725. This work has been authored by a contractor of the U.S. Government, accordingly, the U.S. Government retains a nonexclusive, royalty-free license to publish or reproduce the published form of this contribution , or allow others to do so, for U.S. Government purposes.

Thanks to Dr. Jacob Barhen, Dr. Vladimir Protopopescu, and Dr. David Reister for their assistance and for the use of their research which aided in the development of my project. Thanks to my colleagues Julien Dahan and Gabriel Amselem for their assistance. I would also like to thank Dr. Z.T. Deng from Alabama A & M University for making me aware of this opportunity and for his help in getting me here. Finally, special thanks to Debbie McCoy, Cheryl Hamby, Kathy Rollow and all others who made provisions for this research experience.

Office of Science U.S. Department of Energy

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