Comparison Algorithm for Descent Speeds in Local Minimization Processes for TRUST

Nonlinear optimization problems surface in every field of scientific, technologic, economic or social interests. The objective function to be globally optimized is typically multi-modal, i.e., it possesses many local minima in the region of interest. In most cases, it is desired to find the local minimum at which the function acquires its lowest value, known as the global minimum. 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 [see Barhen et al., *Science*, 276, 1094-1097 (1997)]. The scope of this research is to compare three different methods for reaching local minima. These include conventional gradient descent, conjugate gradients, and a new algorithm based on "fractional power adaptive switching gradient descent" (FPASGD). The rationale is that even a small gain in local minimization will result (potentially) in an exponential gain in the global optimization problem. The focal point of the research will essentially be a comparison of descent speed i.e., the number of iterations needed to obtain a local minimum. The research procedures involved primarily extracting from the TRUST code those algorithms involved in local minimization. These algorithms were altered to produce a code enabling comparison between the three local minimization methods. This process consisted of first establishing the algorithms pseudo code, then editing TRUST such as to retain all needed variables. The final process consisted of testing benchmark functions of multiple variables. Currently, the results show that the FPASGD method reduces the time to reach local minima over the traditional gradient descent method. Work to compare the new technique to the conjugate gradient method is in progress and will be reported prior to project completion. Ongoing applications of TRUST include the study of Lennard-Jones atomic clusters (for DOE) and decision analysis (for NASA). These large scale projects will benefit scientifically and economically from the improved speed in reaching local minima.

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