Amgen Seminar Series in Chemical Engineering

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Derivative-Free Optimization: Algorithms, Software, and Applications

By

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This talk addresses the solution of optimization problems using algorithms that require only the availability of objective/constraint function values but no derivative information. We refer to these algorithms as derivative-free algorithms. Derivative-free approaches can be used for optimization based on simulation or experimental measurements. Fueled by a growing number of applications in science and engineering, the development of derivative-free optimization algorithms has long been studied and found renewed interest in recent years. In this talk, we begin with a review of derivative-free algorithms, followed by a systematic comparison of over twenty related software implementations using a test set of over 500 problems. The algorithms are tested under the same conditions and ranked under several criteria, including their ability to find global solutions to nonconvex problems. To illustrate the potential of these algorithms, we present an application of derivative-free optimization to the protein-ligand conformation prediction problem, for which we find that derivative-free algorithms identify solutions that considerably outperform solutions from the popular AutoDock package. Finally, we propose new local and global derivative-free algorithms that rely on global optimization of algebraic models in surrogate management frameworks for this class of problems.

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