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Comparison of derivative-free optimization methods for groundwater supply and hydraulic capture community problems

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Abstract

Management decisions involving groundwater supply and remediation often rely on optimization techniques to determine an effective strategy. We introduce several derivative-free sampling methods for solving constrained optimization problems that have not yet been considered in this field, and we include a genetic algorithm for completeness. Two well-documented community problems are used for illustration purposes: a groundwater supply problem and a hydraulic capture problem. The community problems were found to be challenging applications due to the objective functions being nonsmooth, nonlinear, and having many local minima. Because the results were found to be sensitive to initial iterates for some methods, guidance is provided in selecting initial iterates for these problems that improve the likelihood of achieving significant reductions in the objective function to be minimized. In addition, we suggest some potentially fruitful areas for future research.

Keywords: Sampling methods; Genetic algorithm; Local minima; Nondifferentiable objective function

1. Introduction

Problems involving the design of groundwater supplies and contaminant containment and removal from subsurface systems can be difficult to solve in anything approaching an optimal fashion. The objective function of interest is often discontinuous, nonlinear, nonconvex, and replete with local minima. Moreover, evaluation of the objective function often requires the solution of an approximate

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numerical simulation model, which can be both expensive and subject to poor resolution of the physical phenomena of concern. Thus, the difficulties of achieving an optimal solution for groundwater supply and contaminant transport problems have their roots in physical aspects of the problems of concern, which are manifest in terms of a challenging set of mathematical characteristics.

Two additional impediments to the advancement of optimal design approaches exist for this class of problems. First, many potential methods exist, but most work focuses on only a small number of available methods for an idealized example problem, which may not have the same range of difficulty as the real class of problems of concern. Second, many optimization methods exist that have yet to be compared and in some noteworthy cases have yet to even be considered by the water resources community.

In response to these observations Mayer et al. [57] proposed a set of so-called "community problems" (CPs), which included a range of supply and remediation problems. The CPs offer a set of challenging and realistic applications to support methods comparison and advancement. An additional hope in introducing the CPs was that the existence of these problems would catalyze the introduction of new methods into the water resource field and perhaps unite subsets of the optimization community by stimulating the joint solution of interesting and difficult problems with a range of methods, which in total would be beyond the reach of any single research group in a reasonable length of time. Overall, it was hoped that the CP would serve to hasten the rate of maturation of optimization methods for important water resources problems and improve the community's ability to arrive at effective designs for realistic problems.

Global solutions to the CPs have not yet been determined or even shown to exist. However, the CPs have received consideration in the literature [32,33], and interest in these problems appears to be increasing in scope and frequency [56,42,39,43]. Two areas in which the CPs have yet to be successful are the introduction of broad new classes of methods into the water resources field by experts in mathematical optimization and comparisons of significant sets of methods for the same problem.

Because the CPs are realistic, they possess many of the mathematical difficulties previously alluded to: they have nonsmooth, nonlinear, discontinuous, nonconvex objective functions that have many local minima. Derivative-based optimization methods are well known to perform poorly on problems with these characteristics, which has given rise to an increase in popularity of genetic algorithms (GAs) [38,44,45] and simulated annealing methods [50] in the water resources field [62,29,19,27], which do not require the evaluation of derivatives of the objective function with respect to decision variables.

Such optimization problems arise in many other areas of science as well [71,15,9]. The mathematical optimization community frequently uses a class of deterministic methods, which we refer to here as sampling methods, to approximate the solution of such problems [71,15,9]. Sampling methods do not require derivatives of the objective function and in general rely upon a direct search of the decision space guided by a pattern or search algorithm. Deterministic sampling methods are a potentially important class of optimization methods which have received only limited use in the water resources literature [10,33,32,42,39,67], and most such sampling methods have yet to be considered at all by the water resources community. These methods are different from commonly used sampling approaches such as GAs in that there is no randomness in the method, and there are rigorous convergence results. We include a very robust GA in the results of this work, so that the deterministic sampling methods can be compared to an approach that is more commonly used in water resources.

The overall goal of this work is to introduce and evaluate several members of an important class of optimization method by solving a subset of the CPs. The specific objectives of this work are: (1) to detail several sampling methods suitable for solving challenging water resources problems, such as the CPs; (2) to evaluate the performance of the sampling methods in terms of the solution achieved and computational effort required for a subset of the CPs as a function of the problem specification and initial conditions; and (3) to provide guidance for selecting an initial iterate for the CPs that improves the performance of the optimizers.

2. Model problems

2.1. Overview

The CPs of concern in this work are a subset of a broad class of problems described by Mayer et al. [57,58]. The CPs consist of model formulations and a wide range of physical domains, objective functions, and constraints for a total of 30 design applications. In the sections that follow, we describe the model problems of focus in this work and specify the hydrologic setting, objective function, constraints, simulator, and method details and links.

2.2. Model problems

We consider two CPs, a water supply problem and a hydraulic capture problem, which are described in Mayer et al. [57,58]. The water supply problem is also described by Fowler et al. [33]. The objective of the water supply problem is to minimize the cost to supply a specific quantity of water subject to a set of constraints. The cost involves installation and operation cost for a set of extraction wells subject to constraints on the net extraction rate, pumping rates, and hydraulic head. The decision variables are the $\{(x_i, y_i)\}_{i=1}^{n}$ locations and pumping rates $\{Q_i\}_{i=1}^{n}$, of the wells, and the number of wells n. We also considered a case in which only the locations of a fixed number of wells pumping at a specified rate were decision variables.

The objective of the hydraulic capture CP is to minimize the cost needed to prevent an initial contaminant plume