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Telescoping strategies for improved parameter estimation of environmental simulation models

L. Shawn Matott[a,*], Beth Hymiak[b], Camden Reslink[c], Christine Baxter[c], Shirmin Aziz[b]

[a] University at Buffalo, Center for Computational Research, 701 Ellicott Street, Buffalo, NY 14203, USA
[b] Buffalo State College, Mathematics Department, 317 Bishop Hall, Buffalo, NY 14222, USA
[c] University at Buffalo, Department of Mathematics, 244 Mathematics Building, Buffalo, NY 14260, USA

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ABSTRACT

The parameters of environmental simulation models are often inferred by minimizing differences between simulated output and observed data. Heuristic global search algorithms are a popular choice for performing minimization but many algorithms yield lackluster results when computational budgets are restricted, as is often required in practice. One way for improving performance is to limit the search domain by reducing upper and lower parameter bounds. While such range reduction is typically done prior to optimization, this study examined strategies for contracting parameter bounds during optimization. Numerical experiments evaluated a set of novel “telescoping” strategies that work in conjunction with a given optimizer to scale parameter bounds in accordance with the remaining computational budget. Various telescoping functions were considered, including a linear scaling of the bounds, and four nonlinear scaling functions that more aggressively reduce parameter bounds either early or late in the optimization. Several heuristic optimizers were integrated with the selected telescoping strategies and applied to numerous optimization test functions as well as calibration problems involving four environmental simulation models. The test suite ranged from simple 2-parameter surfaces to complex 100-parameter landscapes, facilitating robust comparisons of the selected optimizers across a variety of restrictive computational budgets. All telescoping strategies generally improved the performance of the selected optimizers, relative to baseline experiments that used no bounds reduction. Performance improvements varied but were as high as 38% for a real-coded genetic algorithm (RGA), 21% for shuffled complex evolution (SCE), 16% for simulated annealing (SA), 8% for particle swarm optimization (PSO), and 7% for dynamically dimensioned search (DDS). Inter-algorithm comparisons suggest that the SCE and DDS algorithms delivered the best overall performance. SCE appears well-suited for solving low-dimensional problems using a moderate computational budget, while DDS appears better suited for solving high-dimensional problems using a restricted computational budget.

1. Introduction

Environmental modelers must often establish input parameter values given limited site-specific knowledge. Standard practice performs parameter estimation (aka calibration) to infer these unknown values by matching model outputs against corresponding historical data. An optimization-based approach coupling a given model with an optimization search algorithm is commonly employed. The optimizer adjusts model parameter values to minimize a calibration objective function, such as the weighted sum of squared differences between observations and simulated equivalent outputs. Numerous optimizers have been applied to the problem of calibrating environmental simulation models and heuristic global search algorithms are popular choices within the geoscience community (e.g. D'Ambrosio et al., 2006; He et al., 2007; Massoudieh et al., 2008; Matott et al., 2011; Tran et al., 2006; Vesselinov and Harp, 2012; Vrugt et al., 2006). Heuristic optimizers do not use derivatives, instead following empirical guidelines and incorporating structured randomness. These features enable avoidance of three commonly recognized pitfalls encountered during calibration of complex environmental models, namely converging on local minima (Skahill and Doherty, 2006), stalling in insensitive regions (Essaid et al., 2003; Matott and Rabideau, 2008), and difficulty obtaining reliable derivative information (Kavetski, 2006).

Heuristic optimizers can require numerous (e.g. tens to hundreds of thousands) objective function evaluations for good performance. This is impractical for calibrating complex environmental

* Corresponding author. Tel.: +1 716 881 7566; fax: +1 716 849 6656.
E-mail addresses: lsmatott@buffalo.edu, lsmatott@hotmail.com (L.S. Matott), hymiakea01@mail.buffalostate.edu (B. Hymiak), camdenre@buffalo.edu (C. Reslink), cabaxter@buffalo.edu (C. Baxter), saziz207@aol.co.uk (S. Aziz).

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models with forward run-times of minutes to days (Muguntham and Shoemaker, 2006; Mugunthan et al., 2005; Zhang et al., 2009). Practitioners can reduce computational burden by shrinking the parameter space before optimization (e.g. Benaman and Shoemaker, 2004; Johnson and Tucker, 2008; Willms, 2007; Willms and Szusz, 2013). Alternatively, this study introduces several novel strategies for contracting the parameter space *during* optimization.

Five telescoping strategies were developed and explored via extensive numerical experiments. Representative heuristic optimizers were run in a baseline (i.e. no bounds reduction) configuration and re-run using each telescoping strategy. Baseline and modified optimizers were applied to mathematical optimization test functions and environmental model calibration problems involving watershed rainfall-runoff, groundwater flow, and subsurface contaminant transport. Overall, the test suite ranged from easily visualized 2-parameter surfaces to complex 100-parameter landscapes, allowing for meaningful generalization of results. Massively parallel numerical experiments were applied using the test suite, facilitating comparisons of the selected optimizers and telescoping strategies across a variety of restrictive computational budgets.

1.1. Related research

Other approaches for reducing the computational burden of heuristic optimizers include surrogate modeling, parallel computing, model pre-emption, and hybridized algorithms. Razavi et al. (2010) provide a recent review of these approaches, which are complementary to the telescoping strategies developed here. Previous investigations of dynamic range reduction have emphasized a single heuristic optimizer and considered much fewer test problems (e.g. Ndiritu and Daniell, 2001; Nieva et al., 1987; Ryoo and Sahinidis, 1995; Selvakumar and Thanushkodi, 2007; Zamora and Grossmann, 1998). Some existing optimizers already contain operators for dynamically reducing parameter ranges as an essential component of their behavior (e.g. Hansen et al., 2003; Qian and Mahfouf, 2007). However, generalizing these range reduction operators for use within other algorithms is non-trivial. In contrast, the telescoping strategies introduced here are easily linked with arbitrary search algorithms and require no changes to the underlying algorithm mechanics. Heuristic optimizers explored in this research include: a real-coded genetic algorithm (RGA) (Yoon and Shoemaker, 2001), dynamically dimensioned search (DDS) (Tolson and Shoemaker, 2007), simulated annealing for continuously-varying parameters (CSA) (Vanderbilt and Louie, 1984), shuffled complex evolution (SCE) (Duan et al., 1993), and particle swarm optimization (PSO) (Kennedy et al., 2001). This represents a cross-section of available heuristic algorithms.

Calibration methods may be classified as optimization- or uncertainty-based (Razavi et al., 2010). Unlike the optimization-based approach utilized for this research, uncertainty-based approaches delineate distributions of parameter configurations rather than a single optimal parameter set (Marzouk and Najm, 2009; Tarantola, 2005). Uncertainty-based calibration involves the coupling of an environmental or geoscience model with a sampling engine. The sampler randomly generates alternative model parameter configurations with the goal of developing a calibrated probability distribution for the parameters. Tools suitable for uncertainty-based calibration include Generalized Likelihood Uncertainty Estimation (GLUE) (Beven and Binley, 1992), sequential uncertainty fitting (SUFI-2) (Abbaspour et al., 2004) and various Bayesian and Markov chain Monte Carlo (MCMC) implementations (Kuczera and Parent, 1998; Tarantola, 2005). Optimization-based search algorithms are increasingly being incorporated into uncertainty-based approaches (Khu and Werner, 2003; Mugunthan and Shoemaker, 2006; Tolson and Shoemaker, 2008; van Griensven and Meixner, 2007; Vrugt et al., 2006). Thus, the present study is relevant to both types of calibration.

1.2. Parameter estimation in environmental and geoscience modeling

In-depth discussions of calibration in the context of environmental and geoscience modeling are provided elsewhere (e.g. Beven, 2012; Hill and Tiedeman, 2007; Kennedy and O'Hagan, 2001). However a brief review of current practice and challenges serves to highlight the relevance of dynamic range reduction to the geoscience community. As mentioned previously, heuristic optimization is a state-of-the-art approach for parameter estimation that has been widely embraced in the environmental and geoscience modeling communities. With respect to groundwater and subsurface reactive transport applications, the calibration problem is commonly formulated as minimization of a weighted sum of squared residuals expression (Hill and Tiedeman, 2007). In surface hydrology and rainfall-runoff applications, maximizing the Nash–Sutcliffe efficiency measure is a more common objective (Beven, 2012). Data weighting and assimilation schemes also play an important role in the calibration problem formulation (Vrugt et al., 2005), as does the availability and treatment of prior and/or soft information about a given site or case study (Winsemius et al., 2009). Some difficult and somewhat philosophical issues associated with model calibration include: the treatment of equifinality (Beven, 2006; Mantovan and Todini, 2006), the merits of Bayesian and informal approaches to uncertainty quantification (Beven, 2009; Beven et al., 2007; Vrugt et al., 2009), validation methodologies (Konikow and Bredehoeft, 1992; Moriasi et al., 2012; Unger et al., 2012), and multi-model ranking and selection (Poeter and Anderson, 2005; Riva et al., 2011; Ye et al., 2008). These issues continue to be a source of intensive investigation and debate within the environmental and geoscience modeling community.

As illustrated by the preceding overview, calibration of environmental and geoscience models is a complex endeavor with many challenging aspects. However, a common theme among the different approaches and issues is the need to search the calibration parameter space for high-quality or high-probability parameter values. In fact, published procedures for addressing equifinality, uncertainty quantification, validation, and multi-model ranking and selection are all predicated on the ability to identify those parameter sets which provide the best possible correspondence between observation data and simulated responses. By improving search algorithm performance, the telescoping strategies introduced herein facilitate concomitant improvements in many other calibration activities of interest to environmental and geoscience modelers.

2. Methods

The merits of telescoping were assessed via comparison with baseline (i.e. no telescoping) algorithm behavior. Corresponding numerical experiments considered a multi-factored set of treatments including 5 telescoping strategies, 139 test problems comprising variations of 15 mathematical test functions and 4 calibration case-studies, and 5 heuristic optimizers. Mathematical test functions incorporated combinations of 3 alternative computational budgets and 3 levels of parameter dimensionality. Running multiple (e.g. 50) trials of each optimization experiment captured the central tendency of performance.

2.1. Telescoping strategies

Fig. 1 illustrates the general telescoping concept and depicts a two-dimensional objective function surface to be searched by a heuristic algorithm. Parameter bounds are initially assigned a-priori limits (Fig. 1a). As the search progresses, and computational budget dwindles, the searchable parameter bounds are progressively contracted (Fig. 1b–d). In this way the parameter space over