Using Multiobjective Evolutionary Algorithms to Assess Biological Simulation Models

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Abstract. We introduce an important general Multiobjective Evolutionary Algorithm (MOEA) application – assessment of mechanistic simulation models in biology. These models are often developed to investigate the processes underlying biological phenomena. The proposed model structure must be assessed to reveal if it adequately describes the phenomenon. Objective functions are defined to measure how well the simulations reproduce specific phenomenon features. They may be continuous or binary-valued, e.g. constraints, depending on the quality and quantity of phenomenon data. Assessment requires estimating and exploring the model's Pareto frontier. To illustrate the problem, we assess a model of shoot growth in pine trees using an elitist MOEA based on Nondominated Sorting in Genetic Algorithms. The algorithm uses the partition induced on the parameter space by the binary-valued objectives. Repeating the assessment with tighter constraints revealed model structure improvements required for a more accurate simulation of the biological phenomenon.

Keywords: Multiobjective optimization, Pareto frontier, binary discrepancy measures, process model, mechanistic model, model assessment, structural inference, elitism.

1 Introduction

Simulation models are often used to investigate the processes or mechanisms underlying biological or ecological phenomena. For example, the competition process among tree crowns in a dense forest stand was explored by building a spatially-explicit model of crown growth based on simple rules of resource acquisition and utilization at the foliage and branch level [1]. Developing such models involves a considerable degree of uncertainty in the selection of both the model's components and their representation detail. Merely fitting the model to data

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does not guarantee that the proposed model structure adequately describes the phenomenon [2,3]. Rather, the model must be assessed to reveal which aspects of the phenomenon it can produce and which it cannot [2].

Model assessment involves solving a multiobjective optimization problem (MOOP). The model developers select the phenomenon features that the model must reproduce to be considered an adequate system description, then they define an objective function for each feature [2,4]. For example, the crown competition model was assessed for its ability to simultaneously reproduce specific features of tree crown shape and stand level growth rates. The Pareto frontier is then estimated to reveal the model performance tradeoffs among objectives.

This problem can differ from the usual engineering design MOOP in many ways:

- The decision maker is the model developer and the goal is to reveal the inadequacies in the proposed model structure's reproduction of selected features.
- Conceptually, the model is a black-box transforming a parameterization (possible solution) X to a point in the objective space. Model complexity prevents expressing the objective functions directly in terms of X. Rather, the objective functions are expressed in terms of features of the model predictions, $M(X)$. Evaluating a solution X requires running the simulation model, which may be quite computationally intensive.
- Depending on the quality and quantity of data available regarding the phenomenon, an objective function may be a continuous measure of discrepancy between a feature of the model predictions and a target value or simply a binary-valued function evaluating whether the predicted feature falls within an acceptable range [2]. An assessment of a model of stem cell development in cats used six continuous objective functions [5] while the crown competition model was assessed with respect to ten binary objectives due to data limitations [2]. Depending on the objectives, the assessment might be viewed as either a MOOP or a constraint-satisfaction problem (CSP) [6]. However, since the objectives can only be directly expressed in terms of $M(X)$ rather than X, standard CSP methods [6] are inapplicable. We use constraint in the remainder to refer to our nonstandard setting more properly defined as a binary-valued objective function.
- Even if continuous objective functions are used, the model developer will likely summarize the final Pareto frontier by defining an acceptable threshold value for each objective, thus partitioning the Pareto optimal set into sections of the parameter space producing identical constraint satisfaction [2,5].
- The existence of model deficiencies is revealed by (i) constraints that are never satisfied (features not adequately reproducible by the model) or (ii) combinations of constraints that can never be simultaneously satisfied. Maximizing the number of satisfied constraints does not reveal the information required for model assessment.
- Computational demands generally limit model assessments to 4 - 15 objectives and models for which 100,000 complete simulations can be conducted on the order of days to weeks [2,4,5,7].