Evaluation of Advanced Genetic Algorithms Applied to Groundwater Remediation Design

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Abstract

Optimal design of a groundwater pump and treat system is a difficult task, especially given the computationally intensive nature of field-scale remediation design. Genetic algorithms (GAs) have been used extensively for remediation design because of their flexibility and global search capabilities, but computational intensity is a particularly difficult issue with GAs. This paper discusses a new competent GA, the hierarchical Bayesian Optimization Algorithm (hBOA), which is designed to reduce the computational effort. GAs operate by assembling highly fit segments of chromosomes (potential solutions), called building blocks. The hBOA enhances the efficiency of this process by using a Bayesian network to create models of the building blocks. The building blocks are nodes on the network, and the algorithm uses the network to generate new solutions, retaining the best building blocks of the parents. This work compares the performance of hBOA to a simple genetic algorithm (SGA) in solving a case study to determine if any benefit can be gained through the use of this approach. This work demonstrates that hBOA more reliably identifies the optimal solution to this groundwater remediation design problem.

Introduction

In January 2002, the U.S. EPA concluded that pump-and-treat is the most common form of remediation at sites on the National Priorities List with groundwater contamination; there are 700 such sites (USEPA, 2003). There is a substantial capital cost to install wells, as well as an ongoing expense to treat the extracted water. Because these two factors drive the cost of this technology, it is critical to determine the optimal placement and pumping rates of all wells in a timely and cost effective manner.

There is a large body of work that implements optimization techniques on groundwater remediation designs (see, e.g., *Wang et al* 2002, *Papadopoulou et al* 2003, or *Zhi et al* 2003 for examples), and genetic algorithms (GAs) in particular (see, e.g., *Aly et al* 1999*, Bayer et al* 2004, or *Guan et al* 2004 for examples). This work compares three GAs: the simple GA (SGA) that was used in most previous studies, the Bayesian Optimization Algorithm (BOA), and the hierarchical Bayesian Optimization Algorithm (hBOA). It builds on the efforts of Pelikan (2002) and Arst (2002), who found the BOA to be a promising optimization technique. The hBOA is the next generation of BOA, modifying the Bayesian network so that it is more reliable at solving difficult problems. This work investigates the possible gains of using these advanced GAs. The three GAs are evaluated on a hypothetical case study to develop an initial understanding of their behavior.

Case Study Application

The three GAs were tested on a hypothetical case study described by Smalley et al. (2000), and Gopalakrishnan et al. (2003). It is an isotropic, homogeneous aquifer of size 240 x 480 m contaminated with BTEX (benzene, toluene, ethylene, and xylene) at a peak concentration of 200 mg/L. The pumping system allows a maximum of three wells, chosen from 58 possibilities, each with a maximum pumping rate of 250 m^3/day. Of the 58 possible locations, 15 are observation wells. A grid of eight rows by 16 columns was superimposed on the site. The flow of contaminant was modeled by MODFLOW (*McDonald and Harbaugh,* 1988) while the contaminant levels were determined by RT3D (*Clement* 1997*; Clement et al.,* 1998, 2000). Transport includes advection, dispersion, and linear adsorption. Figure 1 depicts this grid, as well as the location of wells and plume concentrations. The optimization problem minimizes the cost of a pump-and-treat technology system subject to a human health risk target, pumping rate constraints, and hydraulic head constraints.

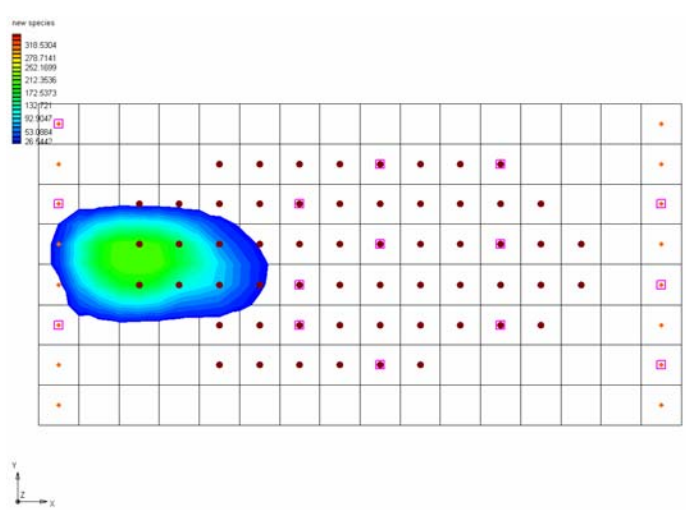

Figure 1: Grid, plume, and well locations for hypothetical case (Source: *Yan*, 2003)

Overview of Genetic Algorithms

The Simple Genetic Algorithm (SGA) (see Goldberg, 1989 for details) was employed as a baseline for comparison of the three algorithms. Two different replacement schemes were used for the SGA in this study. One was non-elitist, and the other elitist. With elitism, the best chromosomes of the parent generation are guaranteed to reach the next generation. In non-elitism, there is no such guarantee. For the SGA without elitism, the children replaced all parents to form the next generation. For the SGA with elitism, the best parent was always included in the next generation.

The BOA operates similar to an SGA initially, randomly generating the initial population and then evaluating it using the objective function and constraints. The BOA employed in this work uses tournament selection without replacement as the selection scheme. Then, a Bayesian network replaces the crossover and mutation steps of a GA. Bits of the chromosome are grouped together, forming building blocks. These building blocks act as the nodes of the network. The algorithm then evaluates the paths through this network, creating new candidate solutions to the problem, as well as identifying the probability that the bits in the building block actually are related. The algorithm creates a joint probability distribution for the building blocks. For the initial population, the prior probabilities are uniform. For subsequent generations, the prior information is the probability that a given set of bits occurred together in the previous generation. Promising solutions are then generated using probabilities from the Bayesian network. The replacement strategy is not elite, as the entire parent population is replaced by the children.

The hBOA method is similar to BOA but, as detailed by Pelikan (2002), several refinements were made to the code. Building blocks still act as nodes on the network. However, a hierarchical element is added to the code. Building blocks are grouped to form larger blocks with a known contribution to the total fitness. In this manner, there are fewer nodes on the network, and it is computationally easier to span the paths of the network.

The drawback to the hierarchical nature of the algorithm is the fact that solutions that have high fitness at a lower level may not necessarily be advantageous at a higher level. This brings about the need to preserve diversity. Building blocks with low fitness at a lower level may be needed at a higher level to achieve an optimal level of fitness. The algorithm includes niching, a process that forces similar chromosomes to compete, as the mechanism to maintain diversity. Since dissimilar chromosomes do not compete, the hBOA will not converge to a single optimal solution as the SGA or BOA would.

Additionally, the replacement strategy in hBOA is unique, employing restricted tournament replacement. In this approach, a subset of the population is randomly chosen. The child chromosome is compared to the specific member of the subset to which it is most similar. If the child's fitness is higher than the parent, then the parent is replaced by the child. This method is not elitist.

Genetic Algorithm Settings

The GA parameter settings for the hypothetical case were based on work developed by Reed (2000) and implemented by Espinoza (2003). Different GA methods may require different minimum population sizes in order to generate reliable results. In order to determine the reliability of each method at different population sizes, three population sizes from the population sizing analysis (see Espinoza 2003 for details) were used: 60, 120, and 240. For all methods at all population sizes, the GA was allowed to run a maximum of 90 generations, but was allowed to stop if 90% of the population has a fitness that is within 0.001% of the best fitness. Since the hBOA does not converge, it was allowed to run for the maximum number of generations that the SGA with elitism ran, 90 generations. To ensure a fair comparison, 20 runs with different random seeds were completed for each GA method at each population size. Each GA method uses the random seed to generate a different initial population.

Results

In order to evaluate the results of each method, a fair method of comparison must be employed. Since the hBOA will not converge, as the other methods do, generations until convergence can not be used. The best fitness for this implementation, the minimum fitness, found in a given generation was the method of comparison chosen. This is not biased against any of the GA methods.

The GA methods varied in the actual number of generations that were executed. This is because some of the methods converged, and some executed for the maximum number of generations. The BOA, at all population levels, converged. The SGA without elitism converged at population levels of 60 and 120, but not 240. The SGA with elitism and hBOA did not converge in 90 generations. Figure 2 lists the maximum final generation for each method at the given population level.

Figure 2: Maximum number of Generations Executed

	Population:		
Algorithm	60	120	240
SGA, not elite	55	81	90
BOA	23	30	39
hBOA	90	90	90
SGA, elite	90	90	90

Figure 3 provides a comparison between GA methods at different population sizes. It shows the best final fitness found by any random seed vs. the number of fitness evaluations needed. At each population size, there is a relatively small difference in fitness between the SGA with elitism and the hBOA for the same number of fitness executions. With the exception of the BOA, the best fitness value found by each method decreases with an increase in population size. Since the BOA always converged, the total number of fitness evaluations for a given population size is always less than that for the other methods. However, the final fitness value is always greater than that for the other methods. This method, with the particular settings used, does not reliably produce an optimal result.

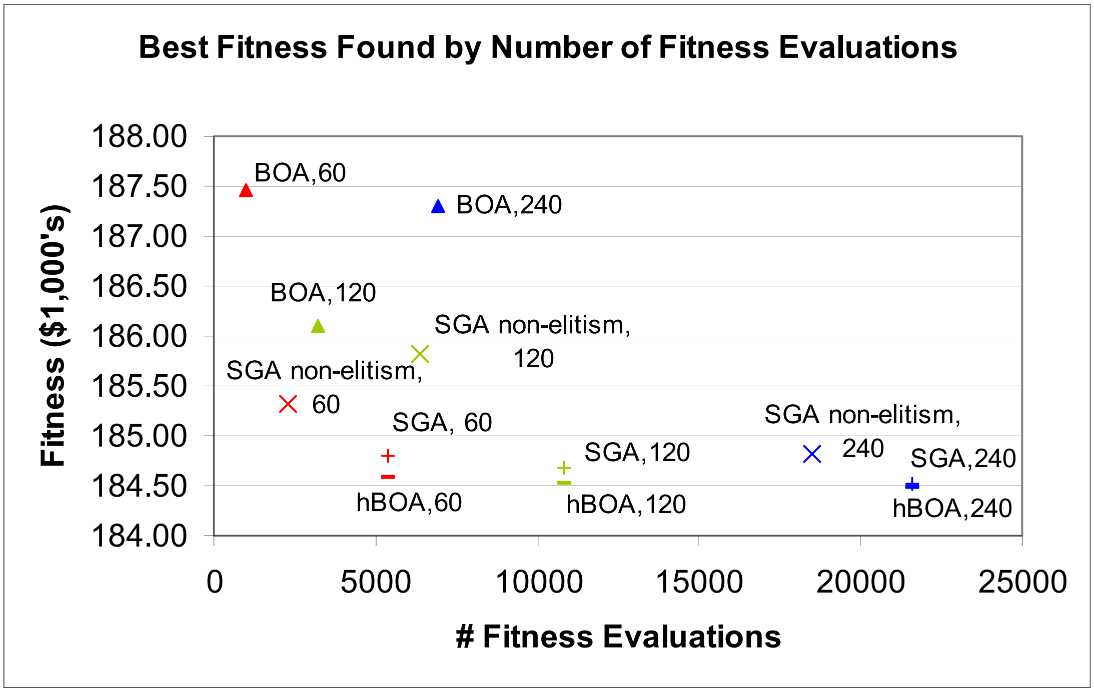

Figure 3: Best Fitness Found for Each Method and Population Size

The range in fitness of the final generation across random seeds can be used as a measure of reliability of the algorithm. By this measure, the hBOA method is shown to be more reliable over all population sizes (see Figure 4). The bars represent the average final fitness (from all 20 random seeds) found by each GA method at a given population size. The error bars on each represent the value of the minimum fitness from the best and worst performing random seeds. The hBOA consistently has a smaller range, making it more reliable. The average final fitness found by the hBOA and the SGA with elitism are relatively close at the two higher population sizes. However, the reliability of the hBOA at the population size of 60 exceeds that of the SGA with elitism. The range of the SGA with elitism is approximately 6.5 times greater than that for the hBOA. It is also apparent from Figure 4 that neither the BOA nor the SGA without elitism approach the optimal fitness.

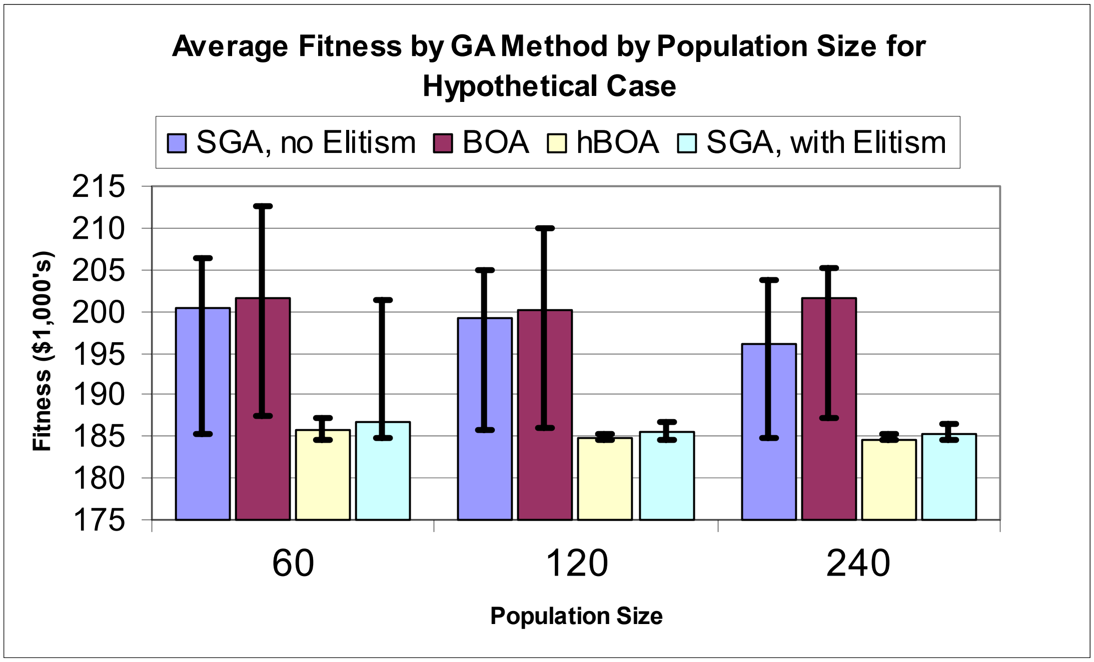

Figure 4: Best, Worst, and Average Fitness over all Random Seeds, by Population Size and GA Method

Figures 5-7 show the average population fitness in each generation for three population sizes and a single random seed. The average fitness of the hBOA has significantly more fluctuations in fitness than the other methods because the hBOA uses niching to preserve diversity of the population. Diversity is necessary because, for so-called "deceptive" problems, good building blocks may not perform well when combined with other building blocks. The improved reliability of the hBOA algorithm indicates that this case study is, in fact, deceptive and the hBOA capabilities are beneficial.

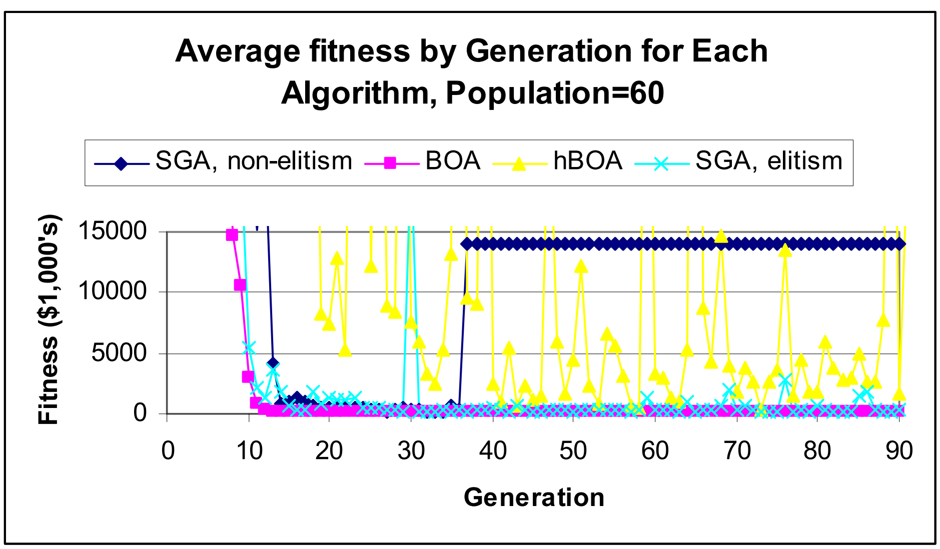

Figure 5: Average Fitness of Each Algorithm, for Population Size 60

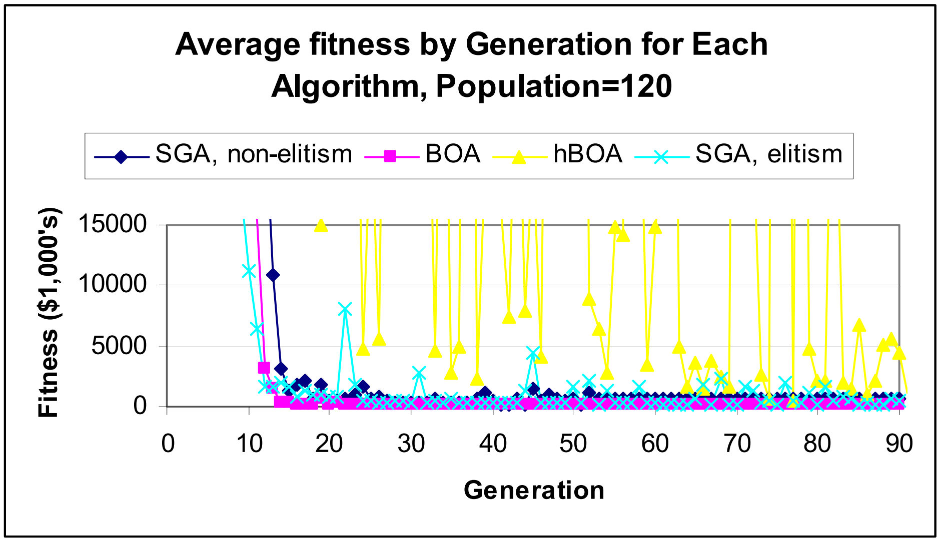

Figure 6: Average Fitness of Each Algorithm, for Population Size 120

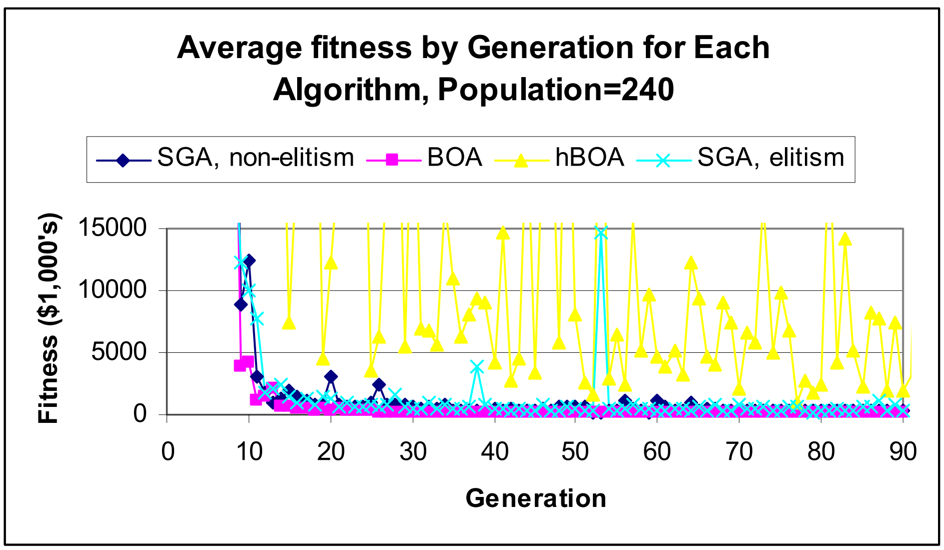

Figure 7: Average Fitness of Each Algorithm, for Population Size 240

Conclusions

This work demonstrates that the hBOA more reliably identifies the optimal solution to this groundwater remediation design problem. The BOA and the SGA without elitism were shown to be ineffective in finding an optimal solution with the settings used. The SGA with elitism also generates reliable results at higher population sizes, but is not able to perform as well as the hBOA at small population sizes. Results from applying the hBOA and the SGA with elitism at a field site will be shown at the conference.

Acknowledgements

This work was supported by the U. S. Army Research Office under Grant No. DAAD19-001-1-0025.

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