Exploration or Convergence? Another Meta-Control Mechanism for GAs

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Abstract
Genetic algorithm based optimizers have to balance extensive exploration of solution spaces to find good solutions with convergence to generate solutions quickly. Many optimizers use a two phase approach where the first phase explores the solution space and the second converges on a set of potential regions. This paper describes a meta-level algorithm (GA ITER ) that iteratively applies a GA based optimizer with a bias towards either exploration or convergence. The optimizer is executed with a very small number of evaluations which leads to fast generation of solutions. The iterative approach of GA ITER has been shown to lead to fast generation of good solutions. Experiments in problems from two real-world domains have shown that GA ITER can improve the performance of an existing GA without compromising the quality of the solution.

Introduction
Optimizers using genetic algorithms have been successfully used to solve many real world optimization problems. This is in part because Genetic algorithms (GA) have proved to be effective at searching a large space of possible solutions and finding good solutions. The issue of how much time or resources an optimizer should expend to find good solutions has been studied for a long time. A consequence of large solution spaces is that optimizers have to deal with convergence on locally optimal but globally sub-optimal solutions. There is a possibility that the population will converge on one particular region of the space. Optimizers need to decide between sampling unexplored regions, i.e., expanding the search, and converging on a subspace. This is a difficult design choice. If an optimizer does not sample sufficient points, it is likely to find itself converging upon a local optimum. On the other hand, an optimizer may over sample the space and it could take a long time before it converges to a good solution. This tradeoff is especially difficult in problems in high dimensional spaces because of the large solution spaces.

This paper describes a meta-level algorithm (GA ITER ) that iteratively applies genetic algorithms to both find good solutions and also converge quickly. On each iteration, the algorithm decides whether to explore (search) or converge (focus) and applies the GA appropriately. The algorithm has been evaluated on problems from two real-world domains, (1) finding the optimal gape (cross-sectional area) of a snake jaw and (2) finding the best set of parameters to model the swimming motion of a pumpkinfish. The first problem involves a search in an eight dimensional space while the second requires a search in a fourteen dimensional space. This paper describes the algorithm along with the experimental results that shows that the GA ITER algorithm significantly improves the performance of an existing GA.

Problem Description
Morphology is the study of how changes in structure can affect function. The jaw of a snake is a complex object composed of many bones and the lengths of the various bones can affect both the size and shape of the prey that can be swallowed. One method of studying the effect is to construct a computational model of the jaw. This section briefly describes the structure of a snake jaw based on a specimen of the gopher snake (Pituophis melanoleucus) and the computational issues involved in studying the morphology.

A snake jaw is composed of ten elements, four bones on each side connected symmetrically by elements at the top and bottom. The four bones on each side are the supratemporal, quadrate, compound and dentary. The elements at the top and bottom are the braincase and symphyseal. Figure 1 is a representation of a snake jaw showing how the elements are connected. In the figure, the braincase and symphyseal are perpendicular to the side view. The symphyseal is not actually a bone but is an elastic element and the amount that it can
be stretched varies from species to species. The joints connecting the elements allow movement in two perpendicular planes, the frontal and the sagittal, for each joint. These movements are constrained by restrictions on the maximum and minimum angles in each plane.

Herpetologists are interested in the size and shape of the largest prey that a snake can swallow. They believe that this is determined by the absolute and relative dimensions of the bones that make up a snake jaw. A snake jaw specification is composed of a set of dimensions for each of the bones. Finding the maximum size of the gape for a jaw specification consists of determining the corresponding set of values for each of the joint angles. This is treated as an optimization problem in eight real-valued dimensions, one for each joint angle subject to (1) constraints on the maximum and minimum values of each joint angle and (2) constraints that the configuration is realizable, e.g., the upper jaw does not overlap the lower jaw. A more detailed description of the problem and the system used to solve it can be found in (Author 2004). The gape is calculated for each configuration as the product of the height (the vertical distance between the upper and lower jaw) and the width (the distance between the left and right quadrate-compound joints. The fitness of a specific configuration is calculated as

\[ csa \times k \times (s - 1) \]  

(1)

where

- \( csa \) : is the cross-sectional area (size of the gape) calculated using the height and width from the model,
- \( s \) : the stretch of the symphseal at maximum gape,
- \( k \) : is the weighting penalty for the use of the symphseal. Stretching the symphseal is viewed as a negative the more the symphseal is stretched, the more the overall merit of the configuration is reduced.

This models the assumption that it is less desirable to stretch the symphseal.

The constraints render many potential solutions infeasible. Figure 2 is a surface plot that shows how the fitness of the solution changes as two of the angles (quadrate-frontal and compound-sagittal) are varied. The plot also shows that there are many infeasible points in the two dimensional region that make it hard to find good solutions in the eight dimensional space.

Several GA based optimization packages including the frequently referenced GALib package (Wall) were tried and evaluated on the snake jaw problem. The GADO (Genetic Algorithm-Based Design Optimization) package (Rasheed, Hirsh, & Gelsey 1997; Blaize, Knight, & Rasheed 1998), an optimization package that was originally developed for the design of supersonic nozzle inlets, was eventually selected for its performance. We systematically varied the parameters for each of the optimization packages and found that the GADO package had the best performance for both time and solution quality. Figure 3 shows a comparison of the best performance of GADO and GALib on an example snake jaw problem. The performance on this problem instance is typical of the performance on other instances.

**Convergence versus Exploration**

The tradeoff between convergence and exploration arises when there is a decision as to whether to generate new (subsequent) points from an unexplored region (exploration) or near a known good point (convergence). A GA should converge when it is in a region that is believed to lead to better solutions. The GA should explore when the current region will not yield significantly better solutions. Two factors that greatly affect the decision as to whether to explore or converge are (1) the total number of points to be evaluated (indirectly, this affects the number of generations of the population) and (2) the size of the population. A GA typically uses...
random sampling (exploration) to fill the initial population pool and then uses a combination of (1) mutation, (2) recombination and selection to generate new individuals for subsequent generations. If the size of the population is too small, the GA will have insufficient diversity to effectively use its operators. On the other hand if the population size is too large, computational resources are expended to managing and analyze the individuals in the population. The total number of points (individuals) to be evaluated also directly affects how quickly a GA can or should converge upon a solution. If the total is relatively large compared to the population size, the GA can initially spend more resources (time) examining (sampling) points from unexplored regions rather than combining individuals from the population (mutation and cross-over). A larger number of sample points would help the GA avoid sub-optimal regions. On the other hand a larger number of evaluations requires resources, an important consideration when the cost of generating each individual is relatively high or when the solution space is large.

There have been many studies (Grefenstette 1986; Eiben, Hinterding, & Michalewicz 1999; Cicirello & Smith 2000) that have explored various combinations of controlling parameters to generate the best performance in GAs. Using the best set of parameters, i.e. the ones that generate the best solutions, usually results in a GA evaluating many points. This can be computationally infeasible if (1) it requires a substantial amount of computation to generate each point and (2) there are many dimensions (parameters) to the problem so the search space is large. The snake jaw problem is an example of such a problem. It takes $3 \sim 5$ seconds to generate each point and there are eight dimensions in the problem. The best settings for GADO ($\text{number of evaluations} = 8000, \text{population size} = 80$) require four hours to generate a solution for one specification of bone dimensions. The computational cost can be reduced by lowering the total number of evaluations but this can negatively impact the solution quality.

Figure 4 shows how the fitness of the solutions changes as the GA generates successive new individuals. The most interesting observation that can be made from the figure is that there are several places where the GA “plateaus”, i.e. successive individuals do not have any impact on the overall fitness. This occurs after about 200 solutions (individuals) have been generated and again after 2000 and 3500 solutions. In addition, after 3500 points, the GA has essentially plateaued and is generating successive points in the same region without significantly improving the quality of the solution.

The performance can be improved if the GA can avoid regions with low potential and instead focus on searching for good solutions in yet unexplored regions. A region rapidly loses potential if successive points generated from that region are not significantly better. The plot in Figure 4 illustrates two related problems with the current approach. Firstly, many solutions have to be generated before the GA can converge on a good solution. Secondly, there are regions where the GA might avoid generating unproductive solutions by changing its focus. What is needed is an algorithm that (1) generates better solutions faster and (2) will not converge prematurely and generate lower quality solutions by dynamically changing the focus between exploration and convergence. The GA\_ITER algorithm has these desired qualities and is described in the next section.

Other approaches to dealing with the tradeoff between exploration and convergence include swarming (Kennedy, Eberhart, & Shi 2001) and scouting-inspired
evolutionary algorithms (SEA) (Pfaffmann, Bousmalis, & Colombano 2004). Swarming focuses more on using the initial sample of points to find good regions of convergence by incrementally searching from a given location. The SEA approach is similar in many ways to our approach but SEA deals more with trying to avoid locally optimal regions automatically, by modulating the search dynamics based on previously generated individuals. The SEA approach was one of the techniques that was systematically evaluated with different parameters but much like GALib, it was unable to generate solutions that were within 40% of the best solutions generated with GADO.

Algorithm Description

The main idea behind our algorithm is an iterative application of the GA where each iteration requires a decision as to whether to converge or explore. The decision is implemented by “seeding” each iteration with individuals from the previous iteration to bias the GA. The result at the end of each iteration, where each iteration is one complete invocation of the GA, is compared with the result from the previous iteration. A subset of the points in the population at the end of the iteration is then used to seed the next iteration. The number of points used to seed is dependent upon whether the improvement in results between the current and previous iterations is above a given threshold. If the improvement is greater than (or equal to) the threshold, the system will continue in the same direction and will seed with the entire population (excluding infeasible points). If the improvement is below the threshold, the GA has found a plateau and the number of points used to seed the next iteration is reduced. This causes the GA to fill the population by sampling points at random. The number of points used to seed the next iteration biases how much exploration is performed. If the GA is still improving the solution by more than the threshold, the search is strongly biased in the current direction by using the entire population. If the GA has found a plateau, the search is biased in the current direction slightly (it might contain the best solution) by using a much smaller number of seed points.

A second key idea is that the number of points to be evaluated on each iteration of the meta-level algorithm is set at a very low value (just slightly larger than the population size). This causes the GA to converge quickly, even to a sub-optimal region. The subsequent iterations will determine whether the algorithm will continue in this region or explore other regions. This focus on a small number of evaluations on each iteration results in good solutions showing up in a small number of iterations and thus a small number of evaluations.

The GA ITER Algorithm

The basic GA ITER algorithm is given below:

1. Set the parameters for the GA to the recommended default values.
2. execute GADO, evaluate the result and calculate the improvement from the result of the previous execution of GADO. If the improvement is greater than or equal to the threshold, then set the value of number of seed points to converge seed points, seed the next GADO execution with number of seed points from the best clusters (see Section for a description of clustering) found in this execution. Repeat step 2.
3. If the improvement is less than the threshold, then GADO has found a plateau. If there has been no improvement greater than the threshold in the last ten iterations, the algorithm terminates. Otherwise, set the value of number of seed points to explore seed points, seed the next GADO execution with points from the best clusters in this iteration and repeat step 2.

The GA parameters used for our experiments in the snake jaw domain are shown in Table 1.

<table>
<thead>
<tr>
<th>GA Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>population_size</td>
<td>80</td>
</tr>
<tr>
<td>number_of_evaluations</td>
<td>200</td>
</tr>
<tr>
<td>converge_seed_points</td>
<td>80</td>
</tr>
<tr>
<td>explore_seed_points</td>
<td>20</td>
</tr>
</tbody>
</table>

Table 1: GA Parameters for Snake Jaw Problem

The population size is dependent upon the number of dimensions in the problem and the default value in GADO is ten times the number of dimensions. Our experiments showed that the default parameters consistently produced the best results with single applications of GADO.

Clustering and Seeding

There are many ways in which points generated from one iteration can be used to seed the next iteration. The best points from the population could be selected but this has the problem of limiting diversity in that the best points could come from one region or cluster of points and the next iteration would be strongly biased towards that cluster. Instead the algorithm uses clusters of points within the population to seed the next iteration. The clusters are defined as points that are separated from each other by a distance that is less than a clustering threshold. This approach has the advantage of not having a pre-defined number of clusters. The value of the variable clustering threshold is currently set at 0.15, a value that has been experimentally determined.
Table 2: Evaluation of GA ITER on Snake Jaw Problem

<table>
<thead>
<tr>
<th>% of Best Fitness</th>
<th>GA ITER (Avg)</th>
<th>Best</th>
<th>Std Dev.</th>
</tr>
</thead>
<tbody>
<tr>
<td>50%</td>
<td>100%</td>
<td>100%</td>
<td>0</td>
</tr>
<tr>
<td>75%</td>
<td>48.7%</td>
<td>25.9%</td>
<td>17.8</td>
</tr>
<tr>
<td>90%</td>
<td>49.8%</td>
<td>29.5%</td>
<td>12.2</td>
</tr>
<tr>
<td>95%</td>
<td>62.1%</td>
<td>45.9%</td>
<td>15.8</td>
</tr>
<tr>
<td>100%</td>
<td>89.9%</td>
<td>81.7%</td>
<td>11.1</td>
</tr>
</tbody>
</table>

to give good results. Once the clusters have been computed, the clusters are ordered by the best fitness value from each cluster and then the points within each cluster are rank ordered by their fitness values. When selecting the points to seed the next iteration, the best point is removed from each cluster in order of their ranking and placed in the pool. The process is repeated until the pool contains number of seed points points.

Experimental Results

The performance of GA ITER was evaluated in two real-world domains. The first domain is the snake jaw problem described in Section. The second domain is to calculate the best values for the parameters of both a fish and fluid model that best describes the swimming motion of a fish.

The first set of experiments involved evaluating GA ITER on many different variations of the snake jaw problem. Each bone’s dimensions was varied by increasing and decreasing it by 10% up to a maximum of 30%. The maximum stretch of the symphysis was also varied between 1 and 2 times the length of the braincase in increments of 0.2. The evaluation of GA ITER is shown in Table 2. The first column shows the fitness of the solution as a percentage of the best known solution. The second and third columns show the number of evaluations GA ITER takes (as a percentage of the number of evaluations taken by GADO) on average and in the best case respectively to achieve the specified solution quality. For example, it takes GA ITER on average 62.1% (and 45.9% in the best case) of the number of evaluations that GADO takes to find a solution that is evaluated at 90% of the best fitness. The fourth column gives the standard deviation of the performance.

The data shows that GA ITER finds good solutions much faster than GADO. This is especially important for problems where (1) the solution space is large and (2) the cost of generating a solution is high. Figure 5 shows a plot of the performance of the two genetic algorithms on a problem instance from the snake jaw domain.

Fish Locomotion Models

The GA ITER algorithm was evaluated on a second real-world domain, that of modeling the swimming motion of a fish, specifically a pumpkinfish. The swimming model (Root et al. 2004) actually consists of two computational models representing (1) the fish and (2) the fluid. Each model has an effect on the other and information must be exchanged between the models for an accurate simulation. The goal is to use the models to compute a swimming motion that most closely resembles the swimming motion of an actual fish over a specified time interval. The fish model is an approximation based on a sequence of stiff rectangular plates connected through hinges. Currently, the model uses eleven plates and twelve hinges.

Images of a swimming pumpkinfish were recorded over a short time interval at the rate of thirty frames per second. The coordinates of several points on the fish body were extracted from each frame and are used to show the body shape changes (changes in the coordinates) as the fish swims. An iterative loop is used to calculate the coordinates of the corresponding points on the fish model. Each iteration corresponds to an image frame. The coordinates of positions of the digital fish body are then extracted for each time interval of the simulation. The computed coordinates are then compared with coordinates extracted from the video of the actual fish. The badness of a particular solution (set of parameter values) is defined by as the sum of the least squares difference between the actual and computed coordinates over the entire time interval (all iterations). In this case, the optimizer is trying to minimize the errors.

The behaviors of the two models are controlled by setting values for fourteen parameters, e.g. the initial positions, velocities and angles for the plates and hinges and the viscosity of the fluid. The problem is defined as an optimization problem in fourteen dimensions where the goal is to find the best values for the controlling pa-
parameters of the models that minimize the difference in motion between the actual and digital fish.

<table>
<thead>
<tr>
<th>GA Parameter</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>population size</td>
<td>140</td>
</tr>
<tr>
<td>number of evaluations</td>
<td>350</td>
</tr>
<tr>
<td>converge seed points</td>
<td>140</td>
</tr>
<tr>
<td>explore seed points</td>
<td>20</td>
</tr>
</tbody>
</table>

Table 3: GA Parameters for Fish Problem

The GA parameter settings used for this problem are shown in Table 3. All the values other than explore seed points were derived by multiplying the corresponding values from the snake jaw problem with a factor of 14/8 (the change in the number of dimensions of the problem). A similar multiplicative factor was applied to the other parameters used by GADO.

<table>
<thead>
<tr>
<th>Percent of Best Solution</th>
<th>GA_ITER</th>
</tr>
</thead>
<tbody>
<tr>
<td>50%</td>
<td>8%</td>
</tr>
<tr>
<td>75%</td>
<td>9%</td>
</tr>
<tr>
<td>90%</td>
<td>10%</td>
</tr>
<tr>
<td>95%</td>
<td>8%</td>
</tr>
<tr>
<td>100%</td>
<td>12.1%</td>
</tr>
</tbody>
</table>

Table 4: Evaluation of GA_ITER on Fish Model

The GA_ITER algorithm performed very well in this second domain. Table 4 shows the data that was obtained for this second problem in comparing the performance of GA_ITER and GADO. Each row shows the number of evaluations taken by GA_ITER (as a percentage of that taken by GADO) to find solutions that are within a certain range of the best known solution. For example, the table shows that to find a solution that is within 90% of the best solution GA_ITER only evaluates 10% of the solutions that GADO examines to achieve the same solution quality. The GA_ITER algorithm is particularly useful in this problem domain because of the computational requirements. Each point (potential solution) takes thirty seconds to generate and using the default parameters for GADO requires a fourteen day computational run. The GA_ITER algorithm finds a good solution (within 5% of the best known) in less than ten percent of the time that GADO takes.

Discussion

The experimental results from the two domains show the GA_ITER algorithm algorithm converges on good solutions much faster than GADO and generates solutions that are just as good. There were some problem instances where GADO had better solutions and other problem instances where the inverse was true. In all cases, the best solution from GA_ITER was within 2% of the best solution of GADO. The combination of (1) the iterative approach with (2) a small number of evaluations per iteration and (3) clustering of points is what makes the approach effective. We have systematically tried clustering and iteration separately but they both lead to little or no improvement.

Conclusion

This paper has described an iterative algorithm for controlling GA’s that provides a better ability to reason and control the tradeoff between exploration and convergence. The algorithm generates good solutions more efficiently, an important factor with problems that (1) have large solution spaces and (2) require significant computational resources to generate solutions. The algorithm has been evaluated on two such real-world problems, one of modeling snake jaws and the second the modeling of the swimming motion of fish.

References


