Sixth International Conference on Artificial Life
Life and Computation: the Boundaries are Changing
University of California, Los Angeles
June 26-29, 1998

ALIFE VI will be held in June of 1998 on the campus of the University of California, Los Angeles, at the Sunset Village conference center, which is a self-contained facility with hotel-style lodging and conference rooms. Over 40 papers will be presented, and approximately 20 posters will be set up for viewing during the conference, with a special demo and poster presentation scheduled for the evening of Saturday, June 27th. In addition, workshops on a wide variety of subjects will be offered during Friday, June 26th, for those who can come early.
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12/12/2000
Artificial Life VI
Proceedings of the Sixth International Conference on Artificial Life
Christoph Adami, Richard K. Belew, Hiroaki Kitano, and Charles E. Taylor, Editors
MIT Press, 1998
(ISBN #0-262-51099-5)

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On the Evolution of Easy Instances

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September 11, 1998

Abstract
We present experimental evidence, based on the traveling salesman problem and
the 2-opt neighborhood, that a genetic algorithm that samples the energy landscape
of an optimization problem and rewards instances that have uniform landscapes,
produces instances that are easy to solve. We discuss possible connections of this
phenomenon to the protein-folding problem.

1 Introduction

The genetic algorithm [8, 10] is a natural, attractive and popular algorithmic idea which, it
is fair to say, has not yet found its compelling application, at least in the realm of combinatorial
optimization (in contrast, simulated annealing, for example, has been demonstrated
to excel in partitioning and VLSI problems [7]). In this paper we identify a natural class
of potential successful applications of the genetic algorithm: Situations in which it is desirable
to construct automatically easy instances of problems. We perform experiments
in which a simple genetic algorithm automatically converges to instances that are rather
remarkable in their simplicity.

Motivation: Protein folding

Our motivation comes from considerations of the protein folding problem. The aminoacid
sequence of a protein typically determines its native state, that is, the unique three-
dimensional shape in which the protein folds with surprising persistence. In turn, the
native state determines the macroscopic properties and function of the protein. It had
been assumed since the 1960s that (a) the native state is the spatial configuration that
minimizes energy, and (b) determining this minimum is a difficult combinatorial problem
—the last assumption was recently verified even in the simplified context of the H-P
model [1, 3]. These two assumptions lead to the so-called Levinthal’s paradox [9, 2]:
How can a protein choose in less than a millisecond among an astronomical number of

1
possible configurations? Or, in view of the recent NP-hardness results, does Nature solve an NP-complete problem? In this note we use computational arguments and experiments to provide an explanation of the alleged paradox which seems plausible both biologically and computationally.

From the computational standpoint our argument is familiar, almost banal: Point (b) above is irrelevant because all combinatorial problems have easy instances. To put it otherwise, although Nature has only a millisecond to solve the instance, it had billions of years to develop the instance. Suppose that we are given a combinatorial optimization problem and a particular “dynamics,” that is, a randomized local search heuristic. Each instance of the problem defines an energy landscape, that is to say, a set of local optima, as well as a distribution over these local optima (Figure 1(a)). Consider now the fitness of this instance to be a measure of the concentration of this distribution, of its closeness to (1,0,0,...) (we give a simple problem-specific example in the next section). Then it is conceivable that fit (“easy”) instances can evolve by a genetic algorithm rewarding fitness; in the next section we present experiments strongly supporting this. Note that this point of view also challenges assumption (a) above: The native state need not be the global optimum, just a hugely popular local optimum (Figure 1(b)).

Sporadic non-algorithmic versions of the above argument can be found in the recent biophysics literature. For example, [11] conjecture that successful proteins have developed efficient “funnels” which facilitate and disambiguate folding, and [5] among others anticipate “metastable” native states that are suboptimal in energy. That uniformity of the folded state of a protein is advantageous to the individual is biologically plausible: Since proteins collaborate in carrying out complex functions by “locking” together geometric features of their native state, protein sequences which persistently fold to the same native state may have an evolutionary advantage over sequences with diverse foldings.
The rigorous way to validate the plausibility of our speculation would be to verify that actual proteins of living organisms have indeed flat energy landscapes; unfortunately this is impossible in view of our current imperfect understanding of the dynamics of protein folding. Instead, we resort to a sort of “computational allegory.” We show that, by sampling the energy landscape of instances of an optimization problem (we use the TSP under 2-opt) and performing random mutations of the instances by rewarding uniformity of the sampling, the instances end up remarkably easy to solve.

2 Experiments

We consider the energy landscape of the Euclidean traveling salesman problem (TSP) under randomized 2-opt (changing two edges at a time, random starting tour, edges considered in random order), and we “evolve” instances of the TSP by a simple genetic algorithm: We start with a population of \( P \) random \( n \)-city instances over the uniform unit square, we sample the energy landscape of each instance \( L \) times (that is, we find \( L \) local optima), and we create the next generation by selecting the \( B \) instances with highest fitness. The fitness of an instance is \( \sum_{1 \leq i < j \leq n} n_{ij}^d \), where \( d > 1 \), and \( n_{ij} \) is the number of local optima in which link \( i - j \) is traversed. The new population contains these \( B \) instances, each perturbed \( P/B \) times by moving each point with probability \( p \), where by “moving” we mean a small normally distributed displacement with standard deviation \( \sigma \).

We varied \( n \) from 20 to 40, 60, 80, 90 and 100 (at which point the procedure became computationally prohibitive, with about a week required for convergence on a Hewlett Packard 712/60 workstation), with at least 10 independent runs for each \( n \) up to 80. All other parameters were optimized experimentally to speed up convergence (typical values: \( d = 2, \ P = 60, \ B = 15, \ L = 40, \ p = .1, \ \sigma = .03 \)). The time requirements can be estimated as \( \Theta(ILPn^2) \), where \( I \) is the number of iterations to convergence. \( I \) appears to grow steeply with \( n \), possibly as a slow exponential of the form \( 2^{\lambda n} \) for some \( \lambda \approx .1 \). In all cases we obtained TSP instances that were (and looked) remarkably easy to solve, essentially “points around a circle.” See Figure 2 for typical 40-city, 80-city, and 90-city final-generation instances.

One possible criticism of this point of view on protein folding is that it disregards function. Fitness cannot depend only on ease of folding, but also on the extent to which the arrived at foldings achieve or approximate favorable shapes. We have introduced such a consideration in a variant of our experiments by rewarding an instance, in addition for the uniformity of its local optima, for the degree to which the local optimal tours resemble a particular tour, say 1,2,\ldots,n,1. Our results here were mixed. Our experiments converged, after a much larger number of iterations, to instances that were rather uniform, but at some distance from the target tour (see Figure 3 for a typical last generation 40-city instance in this experiment). Perhaps better, and more relevant, results could be obtained by considering function (similarity to a given tour) not as part of the objective, but as a constraint on the local optima (this would correspond to insisting that all points
Figure 2: Final-generation TSP instances with 40, 80 and 90 cities.
3 Conclusion and Future Work

Uniformity of the energy landscape is a measure of fitness which is plausible in the case of protein folding, and which experimentally appears to support the evolution of easy solutions in the case of the TSP. Our experiments suggest that the genetic algorithm works remarkably well in optimizing instances, as opposed to solutions — arguably the right genre of problem for this algorithm. Notice finally that the evolution of easy instances may arise in other domains, besides proteins. For example it has been argued (see for example [4]) that innate grammar structures appear to have been optimized for ease of learning.

We are currently experimenting in a similar way with the graph partitioning problem and simple exchange heuristics, and we are obtaining results similar to those we did for the TSP. We are also developing a local search algorithm for the 2-dimensional H-P model for protein folding [2]; the difficulty here is identifying a natural and efficient neighborhood structure (those used by protein scientists working with this model [12] are not appropriate for our purposes). One possible side-product of repeating this experiment in the context of the H-P model could be the discovery of H-P sequences which have a uniquely optimum folding. Such sequences, even of modest length, are very difficult to identify [6].

Acknowledgment: Many thanks to Jon Kleinberg for pointing out to us references [5] and [11].
References


