

Genetic Algorithms, Noise, and the Sizing of Populations

David E. Goldberg

Kalyanmoy Deb

James H. Clark

*Department of General Engineering,
University of Illinois at Urbana-Champaign,
Urbana, IL 61801, USA*

Abstract. This paper considers the effect of stochasticity on the quality of convergence of genetic algorithms (GAs). In many problems, the variance of building-block fitness, or so-called *collateral noise*, is the major source of variance, and a population-sizing equation is derived to ensure that average signal-to-collateral-noise ratios are favorable to the discrimination of the best building blocks required to solve a problem of bounded difficulty. The sizing relation is modified to permit the inclusion of other sources of stochasticity, such as the noise of selection, the noise of genetic operators, and the explicit noise or non-determinism of the objective function. In a test suite of five functions, the sizing relation proves to be a conservative predictor of average correct convergence, as long as all major sources of noise are considered in the sizing calculation. These results suggest how the sizing equation may be viewed as a coarse delineation of a boundary between two distinct types of GA behavior. At small population sizes the GA makes many errors of decision, and the quality of convergence is largely left to chance or to the serial fix-up of flawed results through mutation or other serial injection of diversity. At large population sizes, GAs can reliably discriminate between good and bad building blocks, and parallel processing and recombination of building blocks lead to the quick solution of even difficult deceptive problems. Additionally, the paper outlines a number of extensions, including the development of more refined models of the relation between generational average error and ultimate convergence quality, the development of online methods for sizing populations via the estimation of population-sizing parameters, and the investigation of population sizing in the context of niching and other schemes designed for use in problems with high-cardinality solution sets. The paper also discusses how these results may one day lead to rigorous proofs of convergence for recombinative GAs operating on problems of bounded difficulty.

1. Introduction

An education in genetic algorithms (GAs) begins tamely enough with an initiation to the rites of strings, schemata, selection, genetic operators, and other GA paraphernalia. The first applications to some problem of interest follow in short order, with enough success to justify further experimentation. In the back of the user's mind, however, many detailed doubts and questions linger. How long does it take for GAs to converge, and to what quality answer? What classes of problems can GAs be expected to solve to global optimum? What mix of operators and parameter settings is required to permit such a desirable happenstance? When posed jointly in this fashion, the questions facing the GA community appear dauntingly interrelated and difficult; but starting with Holland's efforts of almost two decades past, and continuing with the renewed interest in GA theory over the last five years, the questions are being divided and conquered through that combination of theory and experimentation appropriate to tackling such complex systems as genetic algorithms.

In this paper we carry on in that spirit of optimistic reductionism, and consider a single question that has puzzled both novice and experienced GA users alike: how can populations be sized to promote the selection of correct (global) building blocks? The answer comes from statistical decision theory and requires that we examine building-block signal differences in relation to population noise. It is somewhat surprising that noise must be considered even when GAs tackle deterministic decision problems, until one recognizes that building-block or collateral noise *is* the cost of parallel subproblem solution within a selective-recombinative GA.

We consider population sizing in the presence of noise by first reviewing six essential elements to GA success. This leads to a brief historical review of past efforts connected with building-block decision making and population sizing. A simple population-sizing equation is then derived, and is used to calculate population sizes for a sequence of test functions displaying varying degrees of nonlinearity, nondeterminism, and nonuniform scaling. This simple sizing equation is shown to be a conservative yet rational means of estimating population size. Extensions of these calculations are also suggested, with the possibility that these methods may be used to develop fully rigorous convergence proofs for recombinative GAs operating on problems of bounded difficulty.

2. A bird's-eye view of GA essentials

When one is mired in a GA run, it is often difficult to discern why things do or do not work. Since Holland's identification of schemata as the unit of selection [30, 31] and specification of a bound on their expected growth [33], a much clearer picture has emerged regarding the conditions necessary for successful discovery. Despite supposed challenges to GA theory that "turn Holland on his head," all known GA results can be explained in purely

mechanistic terms using variations or extensions of Holland's argument; and elsewhere the six conditions for GA success have been itemized [18]:

1. Know what the GA is processing: building blocks.
2. Ensure an adequate supply of building blocks either initially or temporally.
3. Ensure the growth of necessary building blocks.
4. Ensure the mixing of necessary building blocks.
5. Solve problems that are building-block tractable; recode those that are not.
6. Decide well among competing building blocks.

In the remainder of this section, we will briefly review the first five of these building-block conditions, and more comprehensively consider the last.

2.1 Building blocks—the first five essentials

The first three essentials in our list are familiar to most readers of this paper and are not considered further, except to note that the attempts to dress schemata in more elegant mathematical vestment [36, 42] may be considered as special cases of Holland's original (and largely ignored) formulation of schemata as similarity subsets of interacting and hierarchically interconnected finite-state machines [30, 31].

The fourth essential—the issue of mixing—has been little explored, and even in Holland's original monograph it receives only passing mention. Nevertheless, it is certainly the point at which the recent challenges [3, 8, 40, 41] to Holland's call for low-disruption crossover operators will ultimately fall or stand. In this paper we continue to ignore this important issue, except to say that our choice of low-disruption crossover operators and utilization of tight linkage (when necessary) was guided by the recognition that mixing behavior is important to GA success. While the authors just cited have shown that disruption can be reduced sufficiently to permit building-block growth, no convincing evidence of high-order mixing success—empirical or otherwise—has yet been offered. The Second Law of Genetic Algorithms (if one exists) is most certainly a mixing law, but its form has only been hinted at [21, 33]. Further theoretical and empirical study of mixing is underway at Illinois and results from that study will be reported at a later date; whatever the answers to the mixing question are, they will most certainly come from proper application of schema thinking.

Thought along building-block lines has led to the discovery of problems that in an average sense are maximally misleading [7, 11, 13, 14, 16, 34, 43]. Mitchell and Forrest [35] have pointed out that these ideas are not yet fully mature, but the exploration of average-sense deception has led to more challenging test function design. Their fuller exploration is likely to lead us to

better mental models of what makes a problem easy or hard for a GA. The fact that some of these stick-figure models are not fully predictive [27] should not deter us. The give and take of hypothesis formation, experimentation, and hypothesis refinement that is science is leading to a better, more mechanical understanding of GA dynamics. In a more practical vein, it is still an open question whether problems of bounded difficulty can be overcome by obtaining tight linkage on the fly [19], or whether other more sophisticated and effective re-representation operators can be developed to make deceptive problems more amenable to selecto-recombination [34].

2.2 Deciding well

As we better understand the workings of GAs—as we better understand the existence, growth, mixing, and assembly of partial solutions—we are at some point led to consider the accuracy of the decision-making process of selection, as partial solutions are forced to compete with one another. Viewed in this way, choosing between competing building blocks becomes a fairly well-posed problem in statistical decision theory, as was first recognized by Holland [32, 33]. His crucial insight was that implicit parallelism breaks the combinatorially insufferable search for strings into many smaller and more tractable searches for building blocks. Though this division is advantageous in terms of search-set cardinality, it is not purchased without cost. This cost can be demonstrated most dramatically if we compare, in the case of a deterministic search problem, the discrimination between better strings with the discrimination between better building blocks. The problem of determining the better of two strings can be solved with complete confidence through a single pairwise test. At the level of building blocks, despite the determinism of the problem, discrimination becomes an exercise in statistical decision making. This is due to the variation of other building blocks; that is, the simultaneous experimentation with many combinations is a source of noise to any particular building block of interest. It is important, therefore, to control the error in each of the relevant building-block problems that are being played out in a GA if we are ever to have any hope of obtaining a good solution at the end of a run with high probability. If this can be accomplished—and if the other essential conditions of building-block processing can be maintained—then there is hope that convergence guarantees can be determined for simple GAs for which operator probabilities are properly chosen and populations are properly sized.

To make his point about statistical decision making, Holland chose to idealize the process within a GA as a cluster of parallel and interconnected 2^k -armed bandit problems [32, 33]. In attempting to allocate trials to competing alternatives in a sensible manner, Holland viewed the sequential decision process that is played out in realizable GAs in stylized block form assuming perfect foresight, and he calculated an equation relating minimal-expected-loss block size and total number of trials. One may object that realizable GAs are population-wise sequential algorithms, not block algorithms, and

that no realizable GA can know outcomes before they happen—but Holland was aware that his calculation was no more than an optimistic bound on the mathematical form of trial allocation in realizable GAs [32]. Holland was also aware that in realizable GAs many partitions are sampled simultaneously and that the sampling becomes nonuniform after selective reallocation; such awareness did not prevent recent criticism of the bandit idealization [28] on those grounds. Holland's model has been bolstered by recent work that suggests that, because they have higher root-mean-squared (RMS) signal-to-noise ratio values than the lower partitions they subsume, GAs play the highest-order partitions that are well sampled in a given population [24].

Building on Holland's work, De Jong [4] presented equations for the two-armed-bandit block-allocation process that removed Holland's assumption of foresight, and these equations have been solved in closed form fairly recently [12]. De Jong also explicitly recognized the role of signal-to-noise ratio by suggesting that population sizes of order

$$n \geq \frac{\sqrt{\sigma_1^2 + \sigma_2^2}}{|f_1 - f_2|}, \quad (1)$$

where f_1 and f_2 are the mean fitness values, and σ_1^2 and σ_2^2 are the variance values of the two arm-payoffs, respectively, might be useful to reduce statistical decision error. Unfortunately, these calculations were not used to guide the sizing of populations in the largely empirical remainder of De Jong's dissertation.

Elsewhere, the performance of genetic algorithms on noisy functions was studied in the context of image registration [29, 9]. Though largely empirical in nature, this work did recognize the importance of noise in the decision process. However, as the study focused on problems with inherently noisy objective functions, the role of collateral or building-block noise was not considered, and this precluded a more basic understanding of the relationship between noise, resampling, convergence, and population sizing. Nonetheless, the work is one of the few studies since 1975 that has explicitly recognized the role of noise in GA convergence.

One of the motivations for introducing so-called *messy genetic algorithms* or mGAs [21, 22] was to reduce the building-block noise initially encountered during selection and recombination within a simple GA. The earlier of the mGA papers calculated some estimates of fitness variance in typical test functions, and the authors were surprised by the large population sizes that would be required to overcome the collateral noise faced in the typically randomly generated population. More recent work has delved into the relationship between fitness functions and fitness variance using Walsh functions [24, 37], and the thinking found there has led to the development of a population-sizing relation based on signal-to-noise ratio, as well as a suggestion for calculating a variance-adjusted schema theorem. The present study may be viewed as a continuation of that work.

Although not directly related to the present work, several other studies deserve brief mention. Holland's $O(n^3)$ estimate of useful building-block

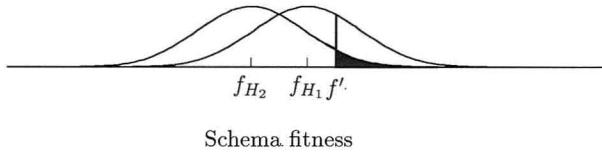


Figure 1: Overlapping distributions of competing schemata permit the possibility of making errors in decisions, especially when only one sample of each schema is taken.

processing is sometimes misconstrued to suggest that building blocks are better processed in larger populations. This notion was debunked [10], and an alternative calculation of the estimate was made available by Fitzpatrick and Grefenstette [9]. Elsewhere [15], population sizing—performed in the context of comparing serial with parallel computations on the basis of schema turnover rate—is applied too literally. That paper coarsely suggests that high schema turnover is promoted with small populations in serial computations and large populations in parallel computations. That result does not contradict the present study, but rather presents an alternative view of the population-sizing question under a different set of assumptions. Here we are concerned primarily with controlling errors in building-block decision making through the use of a large-enough population size—regardless of the type of processor used, and regardless of the real-time rate of schema processing.

3. Population sizing in the presence of noise

Holland [32] set the GA community’s sails on a voyage of stochastic decision making among competing building blocks. We continue along this voyage, ironically making progress by tacking back to a simpler point of departure. Instead of worrying about the form of the optimal allocation of trials over all function evaluations as did Holland [32] and De Jong [4], we simply require that the error in building-block decision making be below some specified level in the first and all subsequent generations. In this way, we expect the GA to make accurate progress with high probability through the normal mechanics of selection and recombination.

3.1 Some basics of statistical decision theory

We start by considering two competing building blocks, call them H_1 (with mean fitness f_{H_1} and fitness variance $\sigma_{H_1}^2$) and H_2 (with mean fitness f_{H_2} and fitness variance $\sigma_{H_2}^2$). We care little how the fitness values are distributed, because given enough samples, the mean fitness approaches a normal distribution as guaranteed by the central limit theorem. Pictorially, the situation we face with a single sample of each of two normally distributed schemata is displayed in figure 1. Clearly schema H_1 is the better of the two, and assuming that the problem is not deceptive (or that we are considering a sufficiently high-order schema that deception is no longer an issue), we hope to choose

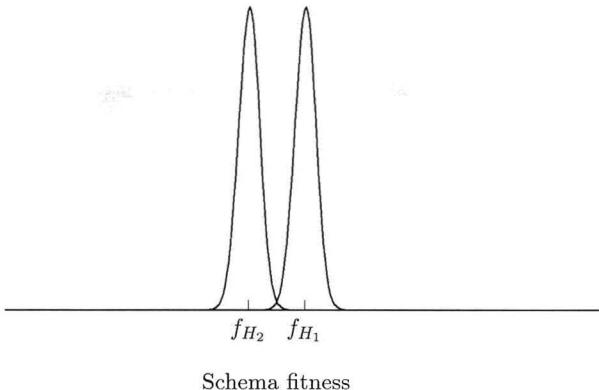


Figure 2: With 25 trials for each schema, the overlap of the distributions of the schema averages is greatly diminished, thereby drastically decreasing the probability of error.

strings that represent H_1 more often than those that represent H_2 . With a single sample in the pictured event, this is not a highly probable situation—as indicated by the overlap in the distributions. In fact, in a single head-to-head comparison of normally distributed H_1 and H_2 , we can calculate the probability that the worse schema of the two is better than a particular fitness value f' , by finding the area of the shaded region. The overall probability that the sample fitness of the second-best schemata is higher than the sample fitness of the best schemata may be calculated by accumulating the above probability for all possible values of f' . This computation is called the *convolution* of the two distributions, and conveniently the convolution of two normal distributions is itself normal: the mean of the convolution is calculated as the difference in the means of the two individual distributions and the variance of the convolution is simply the sum of the individual variances. Thus, defining the *signal difference* $d = f_{H_1} - f_{H_2}$ and calculating the mean variance of the two building blocks as $\sigma_M^2 = (\sigma_{H_1}^2 + \sigma_{H_2}^2)/2$, the probability of making an error on a single trial of each schema may be calculated by finding the probability α such that $z^2(\alpha) = d^2/(2\sigma_M^2)$, where $z(\alpha)$ is the ordinate of a unit, one-sided, normal deviate. Henceforth, we will drop the α and simply recognize z as the tail deviate value at a specified error probability.

If one sample of each building block were all we were permitted, it would be difficult to discriminate between any but the most widely disparate building blocks. Fortunately, in population-based approaches such as genetic algorithms, we are able to simultaneously sample multiple representatives of building blocks of interest. As we take more samples, the standard deviation of the mean difference becomes tighter and tighter, meaning that we can become more confident in our ability to choose better building blocks as the population size increases. This is shown in figure 2, where 25 trials have been assumed for each schema, and the fivefold reduction in standard deviation

results in a much smaller overlap between the two distributions than in our previous example.

3.2 Deriving a population-sizing equation

To put this into practice for particular competitors in a partition of given cardinality, we recognize that the variance of the population mean goes as the variance of a single trial divided by the number of samples. Since the likely number of samples in a uniformly random population of size n is simply the population size divided by the number of competing schemata κ in the partition to which the two schemata belong, the corresponding relationship necessary to obtain discrimination with an error rate α may be written as

$$z^2 = \frac{d^2}{2\sigma_M^2/n'}, \quad (2)$$

where $n' = n/\kappa$. Calling z^2 the coefficient c (also a function of α) and rearranging, we obtain a fairly general population-sizing relation as follows:

$$n = 2c\kappa \frac{\sigma_M^2}{d^2}. \quad (3)$$

Thus, for a given pairwise competition of schemata, the population size varies inversely with the square of the signal difference that must be detected, and proportionally to the product of the number of competitors in the competition partition, the total building-block error, and a constant that increases with decreasing permissible error. The mechanics of a GA, however, involves pairwise competition of a number of building blocks. Thus, to use this equation conservatively, we must size the population for those schemata that may be deceptive and that have the highest value of signal-to-noise-ratio, $\kappa\sigma_M^2/d^2$.

Subsequently, we will generalize this equation to include sources of stochastic variation other than building-block or collateral noise, and will specialize the equation somewhat to get a rough idea of how the population size must change as the deception increases or the problem size grows. At this point we are curious to discover how the coefficient c increases with decreasing error tolerance. Of course, c is nothing more than the square of a one-sided normal deviate. Figure 3 graphs c as a function of error on a logarithmic axis; at low error values, the graph becomes almost linear—as should be expected after straightforward computations involving the usual approximation for the tail of a normal distribution: $\alpha = \exp(-z^2/2)/(z\sqrt{2\pi})$.

3.3 Other sources of noise

The equation derived above is fairly general; however, we have assumed that all the noise faced by the schemata comes from the variance of fitness within the population. Although this is largely true in many problems, GAs may nevertheless face noise from a variety of sources, including inherently noisy problems, noisy selection algorithms, and the variance of other genetic operators. The sizing equation will remain valid, even in cases where these sources

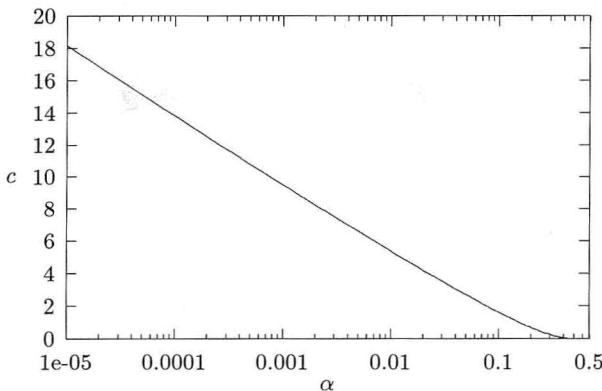


Figure 3: A graph of c as a logarithmic function of error α becomes almost linear at low error rates.

are significant with respect to the collateral noise, if we adjust the variance by including a multiplier for each of the additional sources of stochasticity. For the i th source of noise (call it n_i) with magnitude $\sigma_{n_i}^2$, we can define the relative noise coefficient

$$\rho_{n_i}^2 = \frac{\sigma_{n_i}^2}{\sigma_M^2}. \quad (4)$$

Thereafter, the total additional relative noise coefficient may be calculated:

$$\rho_T^2 = \sum_i \rho_{n_i}^2, \quad (5)$$

assuming statistical independence of all sources of stochasticity, and the modified population-sizing relation may be obtained:

$$n = 2c(1 + \rho_T^2)\kappa\gamma^2, \quad (6)$$

where $\gamma^2 = \sigma_M^2/d^2$, the mean squared inverse overall signal-to-noise ratio. When we examine our initial simulation results, we will demonstrate an appropriate adjustment of the population-sizing equation for Monte-Carlo selection to account for the noise of the roulette wheel. Next, we specialize the general population-sizing equation to functions over χ -ary strings.

3.4 Specializing the sizing equation

The general relationship derived above is widely applicable—perhaps too widely applicable, if one of our aims is to see how the error-limiting population size varies with the difficulty or length of the problem. To understand these factors better we specialize the equation somewhat. Consider strings of length ℓ over alphabets of cardinality χ , and assume that the function

is of bounded deception in that building blocks of some order $k \ll \ell$ containing the global optimum are superior to their competitors. Focusing on the highest order partitions is conservative, and each one contains $\kappa = \chi^k$ competitors. It is convenient (but not necessary) to view the fitness function as the sum of m independent subfunctions f_i , each of the same size k , of the most deceptive partition, thus giving $m = \ell/k$. The overall variance of the function σ_f^2 (in other words, the variance of the most general schema) may be calculated then as the sum of the m variance values:

$$\sigma_f^2 = \sum_{i=1}^m \sigma_{f_i}^2, \quad (7)$$

and we can calculate the root-mean-squared (RMS) subfunction variance as follows:

$$\sigma_{\text{rms}}^2 = \sigma_f^2/m. \quad (8)$$

We then estimate the variance of the average order- k schema by multiplying the RMS value by $m - 1$:

$$\sigma_M^2 = (m - 1)\sigma_{\text{rms}}^2. \quad (9)$$

Using $m - 1$ recognizes that the fixed positions of a schema do not contribute to variance, although the conservative nature of the bound would not be upset by using m . Substituting this value, together with the cardinality of the partition, into the sizing equation yields

$$n = 2c\beta^2(1 + \rho_T^2)m'\chi^k, \quad (10)$$

where $m' = m - 1$ and $\beta^2 = \sigma_{\text{rms}}^2/d^2$, the squared RMS subfunction inverse signal-to-noise ratio.

Assuming fixed c , β , and ρ_T , we note that the sizing equation is $O(m\chi^k)$. If the problems we wish to solve are of bounded and fixed deception (fixed k for given alphabet cardinality regardless of string length), we note that population sizes are $O(m)$; and recalling that $m = \ell/k$, we concluded that $n = O(\ell)$. Elsewhere it has been shown that the typical scaled or ranked selection schemes used in GAs converge in $O(\log n)$ generations [20], and that unscaled proportionate schemes converge in $O(n \log n)$ time. For the faster of the schemes this suggests that GAs can converge in $O(\ell \log \ell)$ function evaluations, even when populations are sized to control error. Moreover, even if we use the slower of the schemes (imagining that the m building blocks converge one after another in a serial fashion, and requiring α to decrease as m^{-1}), GA convergence should be no worse than an $O(\ell^2 \log^3 \ell)$ affair. We will examine the rapid and accurate convergence that results from appropriate population sizing in a moment. First, we need to get a feel for the size of the fitness variance in a typical subproblem.

3.5 Bounds on subfunction variance

Variance of fitness can be calculated directly or through appeal to orthogonal functions [24], but it is useful to have some feeling for the range of fitness variance values we should expect to see in real problems. In a function f of bounded range with specified maximum f_{\max} and minimum f_{\min} , we can calculate the maximum variance of fitness by recognizing that this occurs when half of the strings have the minimum fitness value, f_{\min} , and the other half have the maximum fitness value, f_{\max} . Straightforward computation yields

$$\sigma_f^2 = \frac{(f_{\max} - f_{\min})^2}{4}. \quad (11)$$

With no better idea of the actual variance, using this value as a conservative bound on σ_{rms}^2 in equation 10 is a sensible way to proceed.

If, on the other hand, the function values are nearly uniformly distributed between specified minimum and maximum, a continuous uniform distribution is a good model, yielding a variance of fitness as follows:

$$\sigma_f^2 = \frac{(f_{\max} - f_{\min})^2}{12}. \quad (12)$$

Note that the variance of the worst case is only three times greater than that of the uniformly distributed model.

Taking the argument to the other extreme, suppose we have a function of bounded range, and want to know what the minimum variance can be. This situation occurs in an order- k problem when one of the values is at f_{\min} , one of the values is at f_{\max} , and the other $\chi^k - 2$ values are at the mean. Straightforward computation yields

$$\sigma_f^2 = \frac{(f_{\max} - f_{\min})^2}{2\chi^k}. \quad (13)$$

Of course, this approaches zero as χ or k increases. It is interesting to note that a pure needle-in-a-haystack function with one point at f_{\max} and the remainder at f_{\min} only has a variance of

$$\chi^{-k}(1 - \chi^{-k})(f_{\max} - f_{\min})^2 \approx \chi^{-k}(f_{\max} - f_{\min})^2,$$

which is only a factor of two greater than the minimum variance at high k or χ .

We will use these bounds in the next section, where we apply a simple GA to a sequence of test functions designed to test the efficacy of the population sizing in linear and nonlinear problems, with uniform and nonuniform subfunction scaling, and the presence or absence of explicit function noise.

4. Testing the population-sizing equation

In this section, we test the hypothesis that the population-sizing equation derived in the previous section is a conservative aid to reducing errors in building-block selection. We begin by drawing a somewhat tighter connection between average generational decision error and building-block convergence. We then discuss the design of a suite of problems that test the population-sizing relation across a range of problems that are linear or nonlinear, deterministic or nondeterministic, or uniformly or nonuniformly scaled, and

outline some methodological decisions that were made to both broaden the applicability of our results and simplify the testing. Experimental results for each of the five test functions are then presented, and these support the immediate adoption of the population-sizing relation as a means of controlling convergence error.

4.1 Connection between generational error and ultimate convergence

Earlier we took a generational viewpoint of decision making, and calculated a population size to control the error of decision for a pair of competing building blocks. We have to find our way from this generational perspective to the viewpoint at the end of a run. Calling S the event in which we succeed in converging to the right competing building block at the end of a run, M the event in which we make a mistake in decision making during the initial generation, and C the event in which we choose correctly during the initial generation, we can calculate the success probability as follows:

$$P(S) = P(S | M)P(M) + P(S | C)P(C). \quad (14)$$

By choosing correctly (or incorrectly), we mean that we give more (or fewer) copies to schemata that are actually better (or worse) than some other schema of interest. The interaction between ultimate success and initially correct or incorrect decision making is fairly complex, but we can reason simply as follows. If we choose correctly initially, the probability that we converge correctly is nearly one, because when we make a step in the right direction it is usually a sizable one, and subsequent errors tend to be less frequent than the initial ones and are of smaller magnitude than the correct step taken initially. On the other hand, the greatest chance for making a mistake comes after an initial error, because we have stepped in the wrong direction. Although it is possible (and sometimes even fairly probable) to recover from such initial mistakes, we conservatively ignore such recovery, and get a straightforward bound on ultimate success probability. Setting $P(S | M) = 0$ and $P(S | C) = 1$, and recognizing that $P(C)$ is at least as large as $1 - \alpha$, we obtain

$$P(S) = 1 - \alpha. \quad (15)$$

We define the confidence factor $\zeta = 1 - \alpha$ and plot various convergence measures (usually proportion of building blocks correct) against ζ . Since the chances of getting better than $P(S) = \zeta$ convergence is substantial, the measure of whether the population sizing is conservative will simply be that empirical data fall somewhere above the 45 degree line. In what follows, we call the $P(S) = \zeta$ line the expected lower bound (or expected LB), but we recognize here that it is fairly coarse.

4.2 Test suite design and methodological considerations

To test the population-sizing equation, we consider a simple GA run using various population sizes on a test suite of five real-valued functions (F1 to F5) over bit strings with various levels of stochasticity, nonlinearity, and fitness scaling¹. F1 is a linear function ($\ell = 20, 50, 200$) with uniform scaling. F2 is a linear function ($\ell = 50$) with nonuniform fitness scaling. F3 is a uniformly scaled, linear function ($\ell = 50$) with the addition of zero-mean Gaussian noise. F4 is an order-four deceptive problem ($\ell = 40$) with uniform scaling of the deceptive building blocks, and F5 is an order-four deceptive problem ($\ell = 40$) with nonuniform scaling of the building blocks. More detailed definitions of each function are given in subsequent subsections.

The test suite considers a range of difficulties, and we choose our simple GA carefully to bound the results expected in a range of GAs used in practice. To examine whether the type of selection significantly affects the quality of convergence, we try a number of schemes to begin with, including many of those in wide use. In subsequent tests we restrict our experiments to tournament selection as a good compromise between quality and speed of convergence. In all runs, simple, one-point crossover has been adopted. In linear problems this adoption makes life more difficult for the GA, because of well-known problems with hitchhiking [38]. In nonlinear problems, we have assumed the existence of sufficiently tight linkage to permit building-block growth. As mentioned previously, it is an unanswered question how this may be obtained without prior knowledge, but we did not want to open that Pandora's box, nor the one associated with the adoption of uniform or other highly disruptive crosses. In any event, we are not advocating the use of specific crossover operator here. We simply want to show the effect of choosing well in the presence of collateral or other noise. In all runs no mutation ($p_m = 0$) was used to ensure that initial diversity provided the only means of solving a problem. All runs are terminated when the population converges completely, and all simulations have been performed ten times, each starting with different random-number-generator seeding.

In the remainder of this section, we consider the results of experiments using the population-sizing equation in each of the problems.

¹The term fitness scaling refers to the relative contribution of building blocks in the fitness function.

4.3 Test function F1: A uniformly scaled, linear problem

Linear problems are supposed to be easy for GAs, but most genetic algorithmists have obtained poor convergence in supposedly easy problems at some time when the amount of collateral noise has overwhelmed the signal available. Of course, mutation usually can fix earlier convergence errors in a linear or bitwise optimizable problem, but here we have denied that possibility in an effort to isolate and identify the early decision errors. The initial function chosen to test the population-sizing relation is the uniform linear problem:

$$f_1(\mathbf{x}) = \sum_{i=1}^{\ell} x_i \quad (16)$$

where $x_i \in \{0, 1\}$. This is, of course, the so-called one-max function, and its solution is the string with all ones.

Since the problem is linear, the critical building block is of order one ($k = 1$); the signal we wish to detect has magnitude $1 - 0 = 1$, and the variance of the order-1 building block is simply $(1 - 0)^2/4 = 0.25$, using the variance estimates of a previous section. Thus $\beta^2 = 0.25/1 = 0.25$, and the overall sizing relation becomes $n = c(\ell - 1)$.

To give the GA a good workout, we have tested F1 with a range of string-length values ($\ell = 20, 50, 200$), and a variety of selection operators:

1. roulette-wheel selection (roulette);
2. roulette-wheel selection with ranking (ranking);
3. stochastic universal selection (SUS);
4. binary tournament selection without replacement (tournament).

Roulette-wheel selection is the usual Monte-Carlo scheme with replacement, where the selection probability $p_i = f_i / \sum_j f_j$. Scaled selection scheme uses linear (zero to two) ranking² [1] and Monte-Carlo selection, and the SUS scheme uses the low-noise scheme described elsewhere [2]. Tournament selection is performed without replacement as described elsewhere [20], in an effort to keep the selection noise as low as possible.

Figures 4, 5, and 6 show convergence versus confidence factor (and population size) for $\ell = 20, 50$, and 200 , respectively. Over the range of values, the roulette results are nonconservative (below the expected lower bound), and we will say more about this result in a moment. For the other schemes, the results are barely above the expected lower bound at low confidence values, a not unexpected result because all sources of stochasticity other than collateral noise have been ignored. For the quiet schemes (SUS and tournament), the results become increasingly conservative with increasing n . This increasing conservatism of the sizing relation with increased n is not unexpected. The lower bound relating confidence and ultimate convergence ignores all

²The population is linearly ranked according to the fitness of strings so that the best string is assigned two copies and the worst string is assigned zero copies.

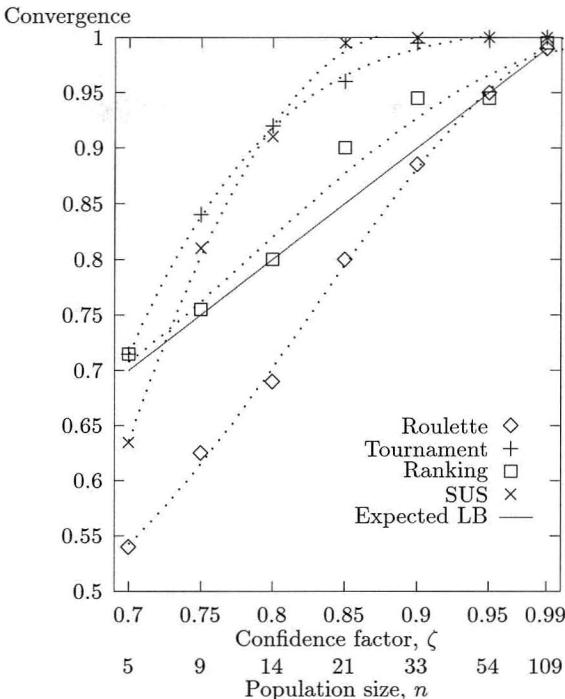


Figure 4: Simulation results for F1 with $\ell = 20$, presented on a graph of convergence as measured by the average number of correct alleles versus confidence and population size. For ζ values greater than 0.7, in all but unranked roulette wheel selection, the graph shows that the sizing equation is conservative even when no additional sources of stochasticity are considered.

possibility of correcting for an initial error. As n increases, drift time for poorly discriminated building blocks increases [25], thereby increasing the probability that a correction can be obtained. A more detailed computation for that mechanism should be sought, but it is beyond the scope of this study. The ranked roulette results stay about even with the expected lower bound for $\ell = 20$ and 50, but have improved margin above the expected lower bound at $\ell = 200$. The previous drift-time mechanism can explain this, with the poor results at lower ℓ values explained by the high inherent noise of roulette-wheel selection itself.

Perhaps the most striking feature of these results is that the roulette-wheel (unranked) traces fall below the expected lower bound. This can be explained by noting that the sizing relation without ρ_T adjustment makes no additional allowance for the noise of selection, and that Monte-Carlo selection with replacement most certainly is a noisy scheme. To quantify this somewhat, let us recognize that n repeated Bernoulli trials are binomially

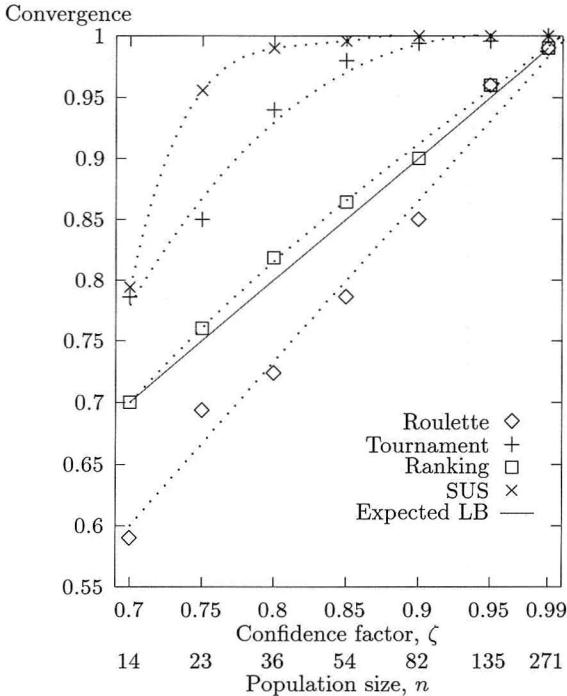


Figure 5: Simulation results for F1 with $\ell = 50$, presented on a graph of convergence as measured by the average number of correct alleles versus confidence and population size. The SUS results at $\ell = 50$ display increasing margin above the expected lower bound when compared with the results at $\ell = 20$.

distributed. Thus, for the i th string, we calculate a mean and variance in the *number of trials* as np_i and $np_i(1 - p_i)$, respectively. Recognizing that $p_i \ll 1$, and summing over all strings, we get a variance $\sum np_i/n = 1$. Thus, the variance in number of trials due to the noise of the wheel is simply one in units of squared individuals. To put this in fitness terms we recognize that an individual must change by an amount equal to the population average fitness to increase or decrease his numbers by one. Thus, the variance due to the roulette wheel in fitness terms is the product of the variance in number times the square of the average fitness (or simply \bar{f}^2). Thus $\rho_T^2 = \bar{f}^2/\sigma_M^2$. Letting $\bar{f} = 0.5(f_{\max} + f_{\min})\ell$, and taking the appropriate variance estimate, $\ell(f_{\max} - f_{\min})^2/4$, we conclude that

$$\rho_T^2 = \ell \left(\frac{f_{\max} + f_{\min}}{f_{\max} - f_{\min}} \right)^2,$$

and in the present case $f_{\max} = 1$, $f_{\min} = 0$, and thus $\rho_T^2 = \ell$. Using this adjustment, we replot the F1 results for the roulette in figure 7, where the

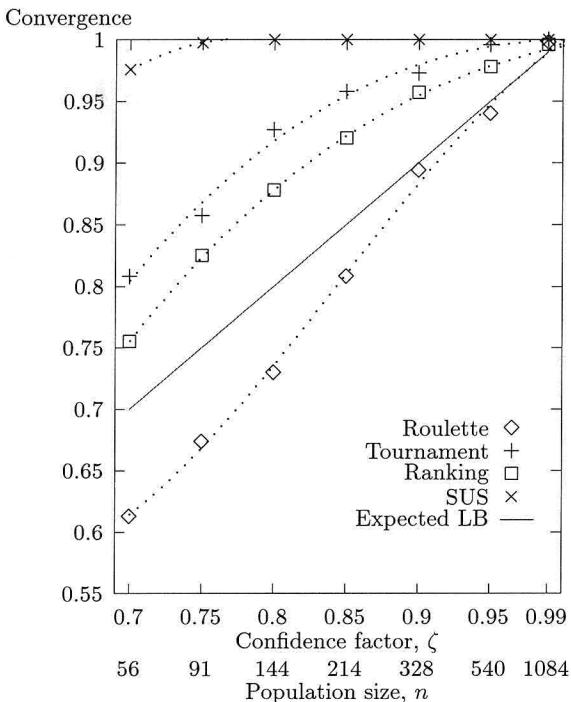


Figure 6: Simulation results for F1 with $\ell = 200$, presented on a graph of convergence as measured by the average number of correct alleles versus confidence (population size). The results are consistent with the $\ell = 20$ and $\ell = 50$ simulations, and the SUS and ranking results show more pronounced margins above the expected lower bound than the runs at lower ℓ values.

existing results have been graphed again using an adjusted α' from the relation $c(\alpha') = c(\alpha)/(1 + \ell)$. The sizing relation is restored to conservatism.

The second most striking feature of the F1 results is the high performance of the two quiet selection schemes, SUS and tournament. This is not unexpected, but the reason for superiority of SUS in most of the cases is unclear without further investigation. Figure 8 shows the total number of function evaluations versus confidence for all schemes and all ℓ values. Clearly, the superiority of SUS is bought at high computational cost. It is well known that purely proportionate schemes tend to slow as average fitness rises [20], but this has a beneficial effect on the quality of convergence, since less pressure is applied to force bad decisions. On the other hand, this tendency increases substantially the total number of function evaluations, and in the remainder of this study we will concentrate on tournament selection as a good compromise between quality and speed of convergence. Looking at the F1 results more closely, we see that for the two pushy schemes (ranking and

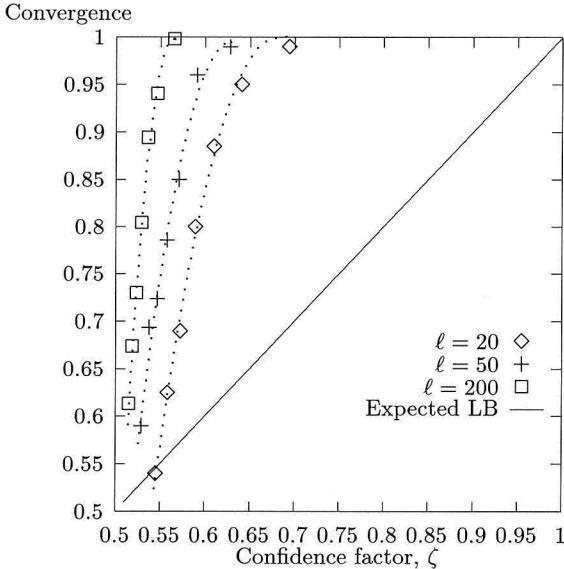


Figure 7: The previous F1 roulette-wheel results have been replotted using a confidence factor calculated after appropriate adjustment for the noise of the roulette wheel. The results are now at or above the expected lower bound.

tournament), the number of function evaluations grows as $\ell^{1.7}$, and for the two purely proportionate schemes (SUS and roulette), the number of function evaluations grows roughly as $\ell^{2.3}$. Recall that ranked and tournament schemes tend to converge in something like $O(\log n)$ generations and that purely proportionate schemes tend to converge in $O(n \log n)$ time [20]; overall, therefore, we should expect a total number of function evaluations of $O(\ell \log \ell)$ to $O(\ell \log^2 \ell)$ for the pushy schemes, which is consistent with the observed $\ell^{1.7}$, and we should expect convergence of $O(\ell^2 \log \ell)$ to $O(\ell^2 \log^3 \ell)$ for the two proportionate schemes, which is consistent with the observed $\ell^{2.3}$. The consistency of these results gives us some hope that these suggestions about convergence and its time complexity can be taken to theoremhood—a matter to be discussed somewhat later in this study. At this juncture, we consider another linear function in which not all bits are created equal.

4.4 Test function F2: A nonuniformly scaled, linear problem

The second test function is also a linear function:

$$f_2(\mathbf{x}) = \sum_{i=1}^{50} c_i x_i, \quad (17)$$

where $x_i \in \{0, 1\}$, $c_i = \delta$ for $i \in I$, and $c_i = 1$ otherwise. Our strategy is

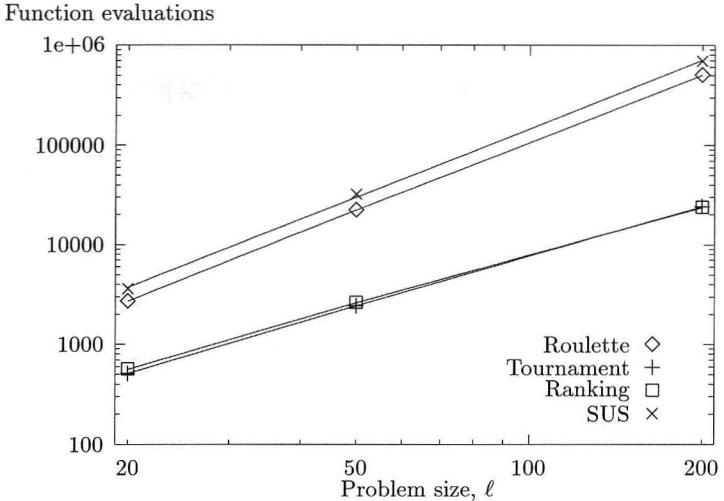


Figure 8: The total number of function evaluations for each selection scheme, graphed versus ℓ value on log-log axes at $\zeta = 0.9$ for function F1. The total number of function evaluations varies approximately as $\ell^{1.7}$ in the pushy (ranking and tournament) selection schemes and $\ell^{2.3}$ in the purely proportionate (SUS and roulette) schemes.

to scale some of the bits badly and observe whether the sizing equation can pick up the small signal amidst the large collateral noise. Among the fifty bits of the problem, only five bad bits are chosen to keep the collateral noise relatively high, and the choice of the set $I = \{5, 15, 25, 35, 45\}$ maximizes the possibility of undesired hitchhiking under single-point crossover.

The sizing of the population is determined as before except that the signal we wish to detect is $d = \delta$. Thus, the population-sizing equation becomes $n = c(\ell - 1)/\delta^2$. As was mentioned, the general success of the sizing formula has encouraged us to continue examination of a single selection scheme, tournament selection. Using tournament selection with all other GA parameters and operators as previously discussed, blocks of simulations have been run for $\delta = 0.4, 0.6$, and 0.8 , and the convergence is shown versus confidence factor in figure 9. Here the convergence measure has been changed to the average proportion of correct alleles among the poorly scaled bits alone. The good bits are well above the noise level, and are extremely unlikely to have any mistakes; including them in the convergence measure gives too rosy a picture. Looking at the figure, the equation proves to be a conservative population-sizing tool in this case as well. In fact, the F2 results are increasingly conservative with decreased δ , a fact that is not surprising due to the extremely conservative nature of the bounding relation we have assumed between generational confidence and ultimate convergence. As n increases, the drift time to incorrect convergence increases linearly, thereby significantly increasing the probability of recovering from initial decision-making errors.

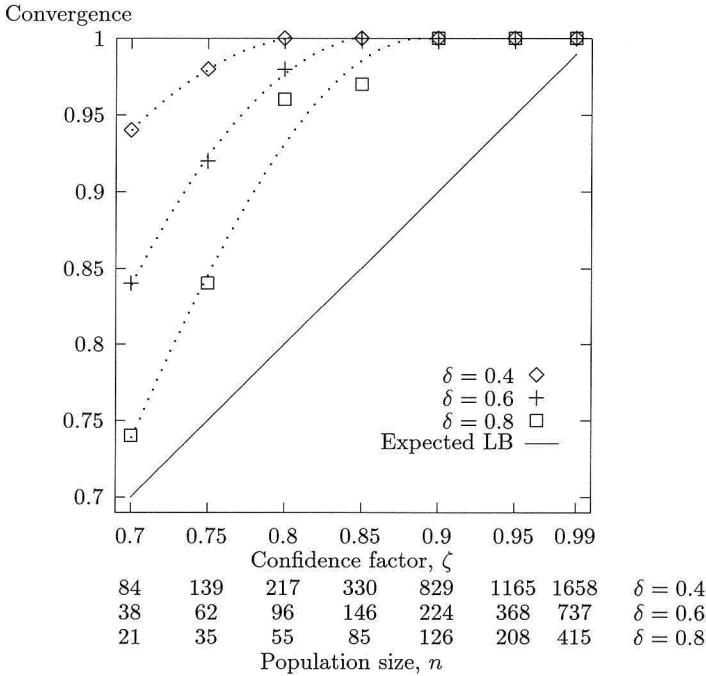


Figure 9: F2 results with $\ell = 50$ show the convergence as measured by the percentage of poorly scaled alleles correct versus confidence at different levels of scaling δ . The sizing relation proves to be a conservative tool in all cases.

4.5 Test function F3: A uniformly scaled, linear function with noise added

For the third test function, we consider another linear function, except this time we add zero-mean Gaussian noise:

$$f_3(\mathbf{x}) = \sum_{i=1}^{50} x_i + g(\sigma_n^2), \quad (18)$$

where $x_i \in \{0, 1\}$ and $g(\sigma_n^2)$ is a generator of zero-mean Gaussian noise of specified variance σ_n^2 .

The sizing relation is the same as in F1, except that a factor ρ_T^2 must be used to account for the noise. Four different levels of noise $\sigma_n^2 = 12.25, 24.5, 49.0$, and 98.0 were added, and these correspond to ρ_T^2 values of 1, 2, 4, and 8.

Convergence (over all bits) versus confidence ζ is shown in figure 10, for blocks of ten simulations on each σ_n^2 - ρ_T^2 case. The sizing relation is conservative in all four cases; as before, increasing conservatism is observed with increasing n .

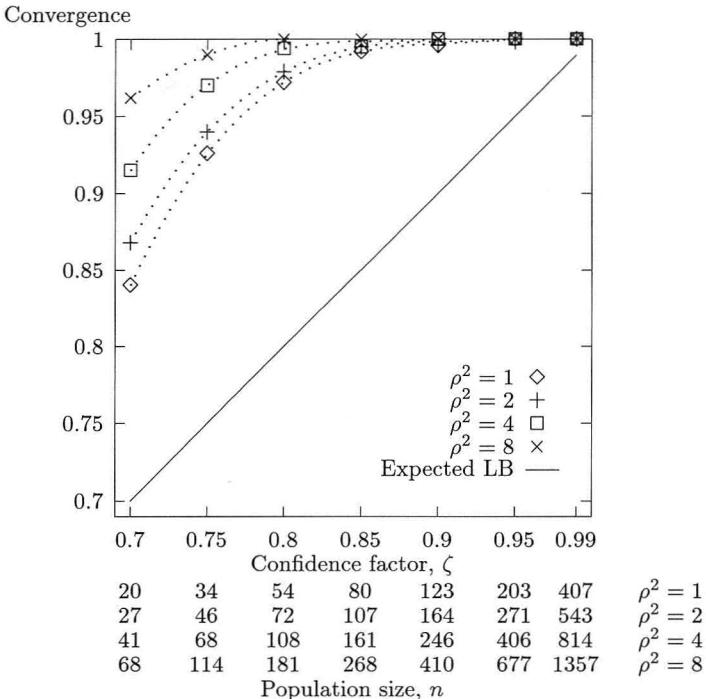


Figure 10: F3 convergence as measured by the average number of ones versus confidence factor, showing that the population-sizing equation adequately handles noisy problems when adjustment is made for the additional stochasticity.

4.6 Test function F4: A uniformly scaled, nonlinear function

In order to study variance-based population sizing in nonlinear problems, a 40-bit, order-four deceptive problem—function F4—has been designed:

$$f_4(\mathbf{x}) = \sum_{i=1}^{10} f_{45}(x_{I_i}), \quad (19)$$

where each of the subfunctions f_{45} is the function shown in figure 11, and the sequence of index sets is the ten sets containing four consecutive integers each: $I_1 = \{1, 2, 3, 4\}$, and $I_{i+1} = I_i + 4$. Function F4 is a function of unitation (a function of the number of ones in the substring argument), and elsewhere it has been shown that this function is fully deceptive in the usual average sense [7]. The variance of the subfunction may be calculated directly and is found to be 1.215. Recognizing that there are ten subfunctions ($m = 10$), that each binary subfunction is of order four ($\chi = 2$, $k = 4$), and that the fitness difference between the best and the second best

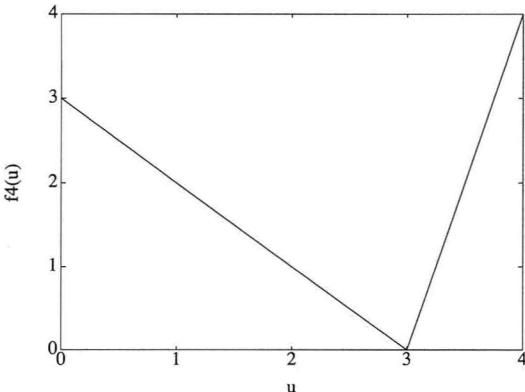


Figure 11: This subfunction is used in functions F4 and F5. Here u is the *unitation* or the number of ones in the subfunction's substring.

substring is one ($d = 1$), the population-sizing equation reduces to $n = 2c(1.215)(10 - 1)2^4/(1^2) = 350c$.

To eliminate building-block disruption as a concern, each subfunction is coded tightly, and tournament selection is used with all other GA operators and parameters set as in previous runs. Figure 12 shows convergence measured by the average number of correct building blocks versus the confidence. Once again the sizing equation conservatively bounds final convergence.

4.7 Test function F5: A nonuniformly scaled, nonlinear problem

To test whether the sizing equation bounds the convergence of a poorly scaled deceptive problem, function F5 has been defined as follows:

$$f_5(\mathbf{x}) = \sum_{i=1}^{10} c_i f_{45}(x_{I_i}), \quad (20)$$

where the subfunction and index sets are defined as in F4, but where the weighting coefficients are no longer uniform. In particular, all the $c_i = 1$ except $c_5 = 0.25$.

Ignoring the minor change in RMS subfunction noise, the sizing of the previous problem may be used as long as it is modified to include the smallest signal. Since the smallest signal that needs to be detected is a quarter of the one of the previous problem, the population size increases by a factor of 16, yielding $n = 5600c$ from the sizing relation.

Binary tournament selection is used as before, and convergence is measured by the average number of correct building blocks, considering only the poorly scaled building block. Starting with $\zeta = 0.7$, in all runs at each value of ζ , the GA converges to the correct (all-ones) string.

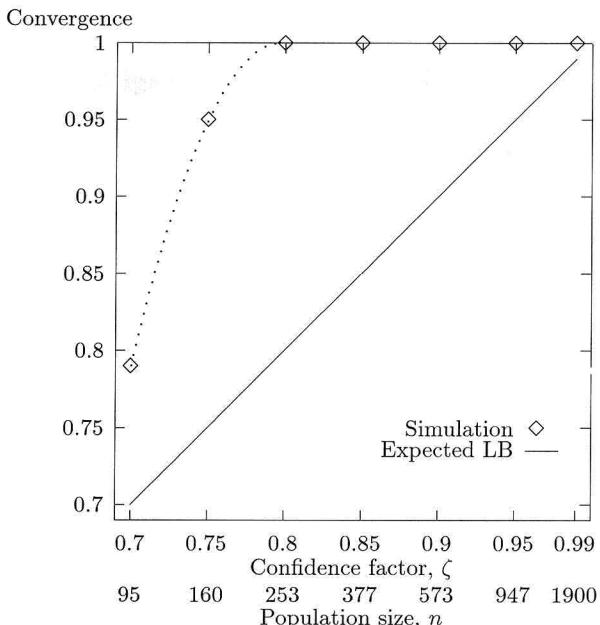


Figure 12: F4 convergence as measured by the average number of correct building blocks versus the confidence factor shows that the sizing equation conservatively bounds the actual convergence in a fairly difficult, albeit uniformly scaled, deceptive problem.

4.8 Summary of results

A population-sizing equation constructed from straightforward statistical decision theory has been used in a number of test problems both linear and nonlinear, from deterministic to inherently stochastic, and with uniform or nonuniform scaling among subfunctions. When additional sources of stochasticity are properly accounted for, the equation appears to be a conservative tool for sizing populations in simple GAs. The population-sizing equation roughly describes the boundary of a transition, at which GAs exhibit a stark change in behavior from noisy and unpredictable convergence to repeatable and reliable results. Moreover, these experimental and theoretical results suggest that if GA convergence can be proved, it is likely to exhibit time complexity that is no worse than quadratic or cubic, depending on the selection scheme used.

These results are useful, and encourage us to seek straightforward proofs of recombinative-GA convergence. There may be objections that the theory is too simple, perhaps suggesting that GAs don't work exactly as the theory idealizes. No model, however, can be placed in one-to-one correspondence, in all respects and in all details, with its modeled object; once this is recognized,

the act of modeling becomes the process of focusing on those aspects of the modeled object relevant to the model's application. Viewed in this way, the sizing relation suggested here captures much of what interests us with no more than a back-of-an-envelope computation. As engineers interested in the design of better GAs, we believe that this kind of modeling should be more widely used. Having said so, we nevertheless do not recommend resting on these laurels, and in the next section we suggest extensions and continuations of this work that will lead to an even deeper understanding of the complex interactions that remain locked away in the population trajectories of even the simplest of GAs.

5. Extensions

The simple population-sizing equation presented in this paper has proven to be a usefully conservative estimate of the population size required to make a controllably small number of building-block errors at the end of a run. Several courses of application and extension readily suggest themselves:

1. Investigate the use of the population-sizing equation on non-binary alphabets, permutation problems, and other codings.
2. Consider the construction of online population-sizing techniques based on these principles.
3. Develop a more fundamental relationship between generational error and ultimate convergence.
4. Investigate in more detail the noise generated by nondeterministic objective functions, selection operators, and other genetic operators.
5. Investigate the interaction of niching and variance-based population sizing in objective functions with multiple global solutions.
6. Investigate other means of forestalling convergence in low-fitness partitions.
7. Use these results to construct computational-learning-theory-like proofs of recombinative GA convergence in problems of bounded deception.

We will briefly examine each of these in somewhat more detail.

The sizing equation deserves immediate testing on other-than-binary codings, although the assumptions used in its derivation are so straightforward that the success demonstrated in this paper could be expected to carry over to other structures without modification. At Illinois we have started to use the sizing relation in problems with permutation operators; our initial experience has been positive.

The sizing relation requires some (albeit minimal) knowledge about the problem being solved, and it may be possible to get online estimates of the necessary values through online population measurements. Specifically, the

sizing relation requires information about the problem size, population variance, minimum signal, and order of deception. Variance may be measured directly and used straightforwardly. Minimum desired signal can be established beforehand, or by keeping track of the change of fitness after a sequence of one-position mutations, an adequate estimate of minimum signal can be given. Order of difficulty is more difficult to measure. Again, a prior limit on the order of maximum deception to be uncovered can be established, or it may be possible to get some estimate of difficulty by doing recursive updates of schema averages or Walsh coefficients as more samples are taken. The schema averages or Walsh coefficients may then be used to see whether there is any evidence of deception in past populations. Once these data are available, the population size may be adjusted in an attempt to control the error of decision, yet keep no more copies than is necessary.

The relation adopted herein between specified error and ultimate convergence is conservative, but it should be possible to develop a more fundamental relation between the two. One thing that aids convergence is that variance in the first generation is something of a worst case. As positions converge, less fitness variance is felt by the remaining competitors, and the environment of decision is much less noisy. Also, as population sizes are increased, convergence is aided, because drift times increase linearly with size [25], and those building blocks in the noise soup—those with relatively unfavorable signal-to-noise ratios—have a longer time to drift around before converging to one value or another at random. It should be possible to construct asymptotic models that more closely relate these effects without resorting to full Markov equations.

This paper has no more than scratched the surface of an investigation of sources of noise other than collateral or building-block noise. Beyond the additive Gaussian noise herein considered lie other noisy objective functions, and representatives of these should be examined to see if the simple variance adjustment is sufficient. The prior expectation is that the adjustment should work, because the central limit theorem works, but the question deserves closer inquiry. Also, the noise generated by various selection schemes should be investigated, as should the noise generated by other genetic operators. We found that the noise of the roulette wheel easily exceeded that of the fitness variance, and this alone accounts for much of the advantage of stochastic remainder selection, stochastic universal selection, and other quieter selection schemes. The variance in operation of the other genetic operators does not affect the sizing as directly as does selection, but it, too, should be investigated. A crossover operator that disrupts a short schema more than expected can be deleterious to convergence and cause errors of decision as well. Similarly, a mutation operator that hits a low-order schema more often than the average can be a problem. These effects should be studied more carefully, and ultimately incorporated into a variance-adjusted schema theorem (a matter discussed as part of the last item).

We have used test functions with singleton solution sets for simplicity. In many problems of interest, the solution has cardinality much greater than

one, and in these problems care should be taken to use *niching* methods [5, 6, 23] or other techniques [17] that permit the stable coexistence of multiple solutions in a population. Such techniques should be used more often, as unbridled competition between species (or corporations) results ultimately in monopoly. This paper also suggests that the same kinds of population-sizing considerations adopted herein should be used for subpopulation sizing within the various niches. Determination of the number of niches is related to the cardinality of the solution set and the ability of the niching criterion or criteria to discriminate between different members of a niche, and, depending on the niching scheme used, some care should be exercised to calculate the fixed-point proportion of members of a given niche properly. If these concerns are addressed, it should be possible to size populations rationally for problems with multiple solutions in a manner not much more difficult than the one used here.

Niching stably preserves diversity across a population, but one of the ways to promote better decision-making in a time-varying environment is through dominance [26, 39] or other *abeyance* schemes. This is particularly useful in the present context for building blocks that fall below the initial signal difference d . Without other protection, selection at these positions is likely to be random affair because of drift; however, if currently out-of-favor building blocks can be protected against cyclical or random runs of bad luck, there is greater hope that when convergence is achieved at a high proportion of positions, these smaller signals can be detected accurately. Dominance-diploidy should be tested to see if low-fitness building blocks can be protected for subsequent competition when the signal-to-noise ratio is favorable. Another possible aid to convergence of low-fitness building blocks is the addition of fitness noise of a scheduled level. This counterintuitive suggestion relates to the observation above that large population sizes prolong drift time for those building blocks that are currently in the noise soup. The injection of noise into a population would insure that low-fitness building blocks would drift and not undergo selective pressure, and large-enough population sizes would insure that those blocks did not drift to absorption. After the first phase of convergence of the highly fit building blocks the noise level could be lowered, thereby exposing the second tier to competitive selection.

Finally, by correcting the decision making in GAs, we feel we have opened the door to straightforward, yet rigorous, convergence proofs of recombinative GAs. It has been pointed out that the schema theorem could be made a rigorous lower bound on schema growth if the various terms were adjusted conservatively for variance effects [24]. We stand by that claim here, and suggest that such results can be pushed further to obtain proofs of polynomial convergence within an epsilon of probability one in problems of bounded difficulty. The actual proofs will resemble those of computational learning theory, and there are a number of technical details that appear fairly tricky, but correct decision making (in a probabilistic sense) is a critical piece of this important puzzle.

6. Conclusions

This paper has developed and tested a population-sizing equation to permit accurate statistical decision making among competing building blocks in population-oriented search schemes such as genetic algorithms. In a suite of five test functions, the population-sizing relation has bounded conservatively the actual accuracy of GA convergence when necessary sources of stochasticity are properly considered and the worst-case signal-to-noise ratio is used in sizing. These results recommend the immediate adoption of variance-based population sizing in practical applications of genetic algorithms as well as more foundational investigations.

The paper has also examined the total number of function evaluations required to solve problems accurately. Convergence appears to be no worse than a quadratic or cubic function of the number of building blocks in the problem (depending on whether purely proportionate selection or more pushy schemes such as ranking and tournament selection have been used). These results are consistent with previous theoretical predictions of GA time complexity, and should open the door to formal proofs of polynomial GA convergence in problems of bounded difficulty, using the basic approach of this paper together with methods not much different from those established in computational learning theory.

Put in somewhat different terms, this paper firmly establishes the role of population size in delineating a boundary between two vastly different types of simple genetic algorithm behavior. At low population sizes we see GAs, converging only through the good graces of random changes that are lucky enough to survive to a time when they may be properly judged. At high population sizes we see GAs that promote only the best among competing building blocks, and when and if these are global, we can expect with high probability convergence to global solutions after sufficient recombination. To understand these two regimes is useful; to have a quantitative yardstick to distinguish high from low population size is important; and to lead these ideas to their logical conclusion is the task ahead.

Acknowledgments

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