
Entropy-Driven Adaptive Representation

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Abstract

In the first genetic programming (GP) book John Koza noticed that fitness histograms give a highly informative global view of the evolutionary process (Koza, 1992). The idea is further developed in this paper by discussing GP evolution in analogy to a physical system. I focus on three inter-related major goals: (1) Study the the problem of search effort allocation in GP; (2) Develop methods in the GA/GP framework that allow adaptive control of diversity; (3) Study ways of adaptation for faster convergence to optimal solution. An entropy measure based on phenotype classes is introduced which abstracts fitness histograms. In this context, entropy represents a measure of population diversity. An analysis of entropy plots and their correlation with other statistics from the population enables an intelligent adaptation of search control.

1 INTRODUCTION

One important problem in search control is the *allocation of search effort*. In general, search effort should be spent to maximize the probability of detection of a solution or to minimize the probability of error or loss. This paper focuses on the definition of extensive state variables, based on statistical measures, that could aid in controlling the allocation of search effort for genetic search procedures such as genetic programming (GP).

Discussing the importance of a statistical theory of evolution, Sewall Wright outlined: “The conclusions favorable to progressive evolution as a process of cumulative change are neither extreme mutation, extreme selection, extreme hybridization, nor any other extreme but rather a certain balance between conditions which make for genetic homogeneity and genetic heterogeneity. Such a situation means on the one hand the retention of a great source of variability in the pop-

ulation and on the other hand a random drifting of the mean grade of all characters, leading occasionally by chance, to the attainment of exceptionally favorable gene combinations” (Wright, 1986).

Genetic heterogeneity, or *diversity*, is one candidate for a useful statistical measure to be considered in this paper. Although the importance of diversity in genetic search is widely recognized in the GA/GP literature, this topic has not been given the deserved formal attention. The notion of diversity has been used mostly in an intuitive way.

The allocation of search effort problem is particularly important in the design of a suitable representation for a new problem. Designing a good representation from the very beginning is a very difficult task. In GP, one usually “throws in” all the basic primitives that are presumed to be necessary in defining a problem solution. Most often the representation of the search space and the genetic operators used to move through the space of programs are not suitable or are biased. It is important to be able to identify such situations and also diagnose how improvements can be achieved.

In this paper we make an analogy between a physical system and the dynamical system represented by a GP population. Under this perspective we look at population entropy and energy as state variables. First, population entropy corresponds to diversity within the population. Population entropy is computed based on a partitioning of the phenotypes into classes. Thus entropy is a state variable that can be observed at negligible computational overload. Second, energy is given by average population fitness.

In order to control the way search adapts to the particular search landscape of a given problem one also needs mechanisms that can vary the behavior of the algorithm as reflected in the state variables or statistical measures considered. Such mechanisms would then define adaptive control criteria in the search effort allocation problem and would help improve the overall behavior of the algorithm. One mechanism of controlling entropy and energy variation is the definition of

subroutines. This paper shows that the correlation between energy and entropy can be successfully used to decide when to create or modify old functions in order to speed up genetic search.

2 APPROACHES TO THE SEARCH EFFORT ALLOCATION PROBLEM

The search effort allocation problem is essentially analogous to the *exploration-exploitation tradeoff*. Application domain heuristics are most often employed to address the problem.

An early attempt to formalize this problem is the “two armed bandit problem” which nicely points out the idea of a tradeoff. The “Two armed bandit problem” was concerned with the allocation of trials to two random variables that offer unitary payoff with unknown probabilities, so that cumulative payoff is maximized (Holland, 1992). Holland outlined that at any given time only one of the following strategies can be pursued: exploit the observed best, which runs the risk of perpetuated error or explore for new information which runs the risk of a performance loss. The solution to the problem essentially shows that the trials allocated to the random variable with the highest observed expectation should be exponentially increased relative to the number of trials allocated to the second variable.

The solution to the “two armed bandit problem” justifies the fitness proportionate reproduction strategy of a genetic algorithm. Under such a strategy, a GA increases the proportion of above average schema (which play the role of the random variables) at a geometric rate, suggesting that the allocation of search effort towards good population schema is close to optimal. This result is formally presented in the GA theory under the name *schemata theorem* and is also placed at the basis of the building block hypothesis in GAs. The building block hypothesis (Holland, 1975; Goldberg, 1989) states that GA achieve their search capabilities by means of “block” processing. Blocks are small schemata representing relevant pieces of a solution that can be assembled together in order to generate problem solutions.

Another expression of the exploration-exploitation problem appears in the reinforcement learning paradigm. An agent chooses its current action in his interaction with the environment in order to maximize future discounted rewards (Watkins, 1989). If the search process chooses the action prescribed by its current knowledge, then the system *exploits* its current knowledge by acting in order to gain reward. It occasionally explores actions at random in order to experiment with more state-action pairs and eventually

improve its policy. If the search process acts to gain information or experience then it *explores* the search space. In the reinforcement learning literature, this tradeoff is made explicit by the control structure of the algorithms.

Iterative improvement search algorithms used in combinatorial optimization (Papadimitriou and Steiglitz, 1982) attempt to improve search control by distinguishing between local and global search regimes and applying heuristics to decide where and how to search next. Local search is search performed in a *neighborhood* of a feasible search space point or configuration. A search neighborhood \mathcal{V}_i contains of all configurations that can be reached from i in a single transition. The choice of the neighborhood depends critically on the structure of the domain of feasible points and is subject to various heuristics, specifying the size and type of the neighborhood, the order to move in the neighborhood, the acceptance criterion (specifying when an improvement is accepted) etc. (Papadimitriou and Steiglitz, 1982) The search effort is specified in terms of bounds on the complexity of the algorithms.

In contrast to iterative improvement algorithms, simulated annealing search algorithms accept cost increasing transitions with non-zero probabilities (Kirkpatrick et al.,) depending on a temperature parameter, in order to avoid the traps represented by local minima. Although simulated annealing present the nice theoretical property of convergence towards global optimum under certain conditions, they practically converge very slowly (Laarhoven, 1988).

A learning system should have an adaptive policy of balancing exploration and exploitation. Such an adaptive policy is possible in GP with subroutines, also called hierarchical GP (HGP) (Rosca and Ballard, 1995).

HGP extensions, such as Automatic Discovery of Functions (ADF) (Koza, 1992) or Adaptive Representation (AR) (Rosca and Ballard, 1994), are based on the discovery, modification and use of new functions (subroutines) to accelerate evolution (Rosca, 1995). Theoretically, HGP approaches allow to scale up genetic programming (GP) applications (Koza, 1994) but practically they face two important problems that confine their efficiency. The “when” problem is that HGP does not employ *informed* choices to decide *when* creation or modification of functions is advantageous or necessary. The “what” problem is that HGP does not automatically decide *which* blocks of code or functions may be worth giving special attention. Essentially, the definition and use of new functions enables the inheritance or exploitation of structures preserved in the population while mutation or crossover determine an exploration of the search space of programs. Crossover usually has drastical effects, depending on the position of crossover points in the function hierarchy. This is a general problem of the GP represen-

tation called *causality* in (Rosca and Ballard, 1995): A “natural” perturbation of a feasible solution (as in (Papadimitriou and Steiglitz, 1982)) is not necessarily a smooth one in the fitness landscape. We could make the GP search engine more efficient by teaching it when to employ subroutine definition and what types of crossover to favor in various search phases.

3 COMPUTATIONAL EFFORT IN GP

(Koza, 1994) estimated the computational effort needed to find a solution with a given probability z as being the minimum number of individuals processed in a number of runs R and a number of generations i which determine a corresponding cumulative probability of success $P(i)$ after i generations:

$$E(z) = \min_i \{M \cdot (i + 1) \cdot R\}$$

where $R = R(z)$ is given by the relation:

$$z = 1 - [1 - P(i)]^R$$

and M is the population size (constant). $P(i)$ is determined experimentally from a sufficiently large number of runs.

In many practical problems solution approximations are desired and the GP success predicate may never get satisfied. In the general case, one is interested in the computational effort needed to reach a percentage x of an ideal solution with a probability z , where $E(x, z)$ is defined as above and $R = R(x, z)$. A generalization of the above analysis to account for this case is straightforward. A sufficiently large number of runs is needed to compute a table for the cumulative probability $P(i, x)$ to reach fitness level x with a given probability z , for a desired z and varying x and i . We obtain:

$$E(x, z) = \min_i \{M \cdot (i + 1) \cdot \lceil \frac{\log(1 - z)}{\log(1 - P(i, x))} \rceil\}$$

Measures such as computational effort $E(\cdot)$ are useful for validation of results, i.e. to analyze, a posteriori, how GP performed. The $E(\cdot)$ measure can not be used as adaptive criteria during the GP search process. For instance, $E(\cdot)$ is useless in deciding how search effort is to be spent in the next generations. It would be useful to define posterior distributions on state variables of interest and to pose the allocation problem in terms of optimization problems on those variables.

4 ANALOGY WITH A PHYSICAL SYSTEM

Ludwig Boltzmann introduced the distinction between micro state and macro state which enabled him to give a statistical interpretation to thermodynamics (Thompson, 1988). The micro state description of a physical system would include a specification of state variables (such as position and velocity) for each particle. Theoretically, this could completely define the state of the system. In contrast, a macro state is a macroscopic description, i.e. one that is defined in terms of observable properties of the system (such as mass, volume or velocity).

In general one can not know the micro state of a physical system. The system’s micro state fluctuates dynamically between micro states consistent with the system’s macroscopic description. Given a micro state there is no way of knowing which particular micro state is producing it.

By analogy to a physical system, consider that the macro state of a stochastic system represented by a GA/GP is defined by its entire population at a given time. We can observe properties that define global measures such as *average fitness* or *best-of-generation fitness*. In GP in particular, many genotypes may correspond to the same phenotype. We may not be interested exactly in which of those genotypes are actually realized. In this analogy, a particular genotype would correspond to a micro state.

We extend the analogy by interpreting fitness as energy. The energy of an individual i is in this case:

$$H(i) = Std-fitness(i)$$

The principle of natural selection is strongly tied to the idea of energy, as individuals in a population compete for the effective utilization of energy resources (Wicken, 1988).

Ideally, there would be no uncertainty regarding the state if the entire population were made up of copies of a single individual (one having the minimum energy for a global optimum state). However, genetic search starts with a randomly generated state. During genetic search micro states fluctuate determining a variation of the state in time (i.e. with generation number).

In thermodynamics, the energy of a system depends on the absolute temperature T , another macroscopic state variable. We may also use temperature in our interpretations. However, in this paper we will only consider that the temperature has a constant fixed value T .

The above analogy enables us to apply some of the results from statistical mechanics in order to qualitatively interpret state changes and convergence in a genetic algorithm, in particular in genetic programming.

The probability of a state i in thermal equilibrium is given by the Boltzmann-Gibbs distribution:

$$Prob(i) = p_i = Z^{-1} e^{-\frac{H(i)}{T}}$$

where Z is a normalizing constant needed in order to make p a probability distribution. Z actually plays a very important role in statistical physics and is called the *partition function*:

$$Z = \sum_i e^{-\frac{H(i)}{T}}$$

If we define the *free energy* of the system as

$$F = -T \cdot \log Z$$

it can be easily showed that

$$F = \langle H \rangle - T \cdot S \quad (1)$$

where $\langle H \rangle$ represents the average value of a random variable H and S is the *entropy* of the system:

$$S = - \sum_i p_i \cdot \log p_i \quad (2)$$

The free energy can be interpreted as the sum of the probabilities of individual states, according to the following identity:

$$\frac{e^{-\frac{F}{T}}}{Z} = \sum_i p_i = 1$$

In the free energy formula (1), estimations of H and S would result in an estimation of F which can be interpreted as the probability of finding the system in a subset of states (Hertz et al., 1991).

In the next chapters we discuss various interpretations of entropy, relate sampled entropy with diversity and show how diversity and energy are correlated in restricted free entropy.

5 ENTROPY AND INFORMATION MEASURES

Entropy is an extensive property of a system's state meaning transformation. The classical interpretation comes from thermodynamics: The entropy function was introduced by Clausius to represent the change of state when an increment of energy is added to a body as heat during a reversible process. It was later interpreted statistically by Boltzmann. The entropy of a system whose micro states are uncertain and have probabilities of occurrence p_i dependent on energy is given, up to a constant, by relation (2). The entropy has a maximum value when all micro states

are equiprobable. Entropy represents the disorder in the system of particles and tends to increase for irreversible processes as the ones in nature, according to the second law of thermodynamics (Thompson, 1988).

Shannon used the same formula to define an information measure representing one's ignorance of which of a number of possibilities actually holds, given the a priori probability distribution represented by P (Shannon, 1949).

Yet another interpretation of entropy is complexity (Chaitin, 1987) or information content of an individual structure. In this context order means compressibility. Redundancies subtract from an individual's complexity.

All these interpretations use the same formula (2) but assign different meanings to the probabilities fed into the formula.

This generalization tendency in interpreting entropy led researchers to search for an unifying view between the statistical interpretations of the second law of thermodynamics in physics and evolutionary principles in biology (Bruce H. Weber and Smith, 1988). Schrödinger (Schrödinger, 1945) and others have noticed the following paradox: The increase in entropy in physical systems brings about a disorganization of the systems. Equivalently, systems evolve from less probable to more probable states. In contrast, natural evolution is described as progress, transformation from simple to complex or from more to less probable states. Schrödinger explained the paradox by looking at the flux of energy in a living system and suggesting that it does not conform to the basic assumptions of classical thermodynamics.

However, there are various claims about the role of the second law of thermodynamics in biological evolution (Bruce H. Weber and Smith, 1988). For instance Wicken proposed that genetic variation is due to the probabilistic nature of the second law (Wicken, 1988). One measure that quantifies variation is *diversity*. Johnson defined diversity in terms of the distribution of the energy within the system based on Shannon's information entropy measure, but outlined that diversity is not perfectly synonymous with either information or with statistical entropy (Johnson, 1988).

6 DIVERSITY

A rule of thumb in the GA literature postulates that population diversity is important for avoiding premature convergence. The problem is how to capture heterogeneity. A straightforward definition of diversity or non-similarity for GA string-based representations is based on the Hamming distance between encodings of individuals.

(Eshelman and Schaffer, 1993) discusses strategies for maintaining GA population diversity by controlling how mates are selected, how children are created by recombination and how parents are replaced. Eshelman and Schaffer propose a method called “incest prevention,” in which individuals are randomly paired for mating provided that their Hamming distance is above a certain threshold. Their method is showed superior in examples based on elitist selection.

In GP, diversity may be defined as the percentage of structurally distinct individuals at a given generation. Two individuals are structurally distinct if they are not isomorphic trees. However, such a definition is not practically useful. It is computationally expensive to test for tree isomorphisms. Moreover, associativity of functions is extremely difficult to take into account. In contrast, similarity between structures can be easily tested in GAs.

(Ryan, 1994) uses an intuitive measure of diversity, based on performance, and shows that maintaining increased diversity in GP leads to better performance. His algorithm is called “disassortative mating.” It selects parents for crossover from two different lists of individuals. One list of individuals is ranked based on fitness, while the other is ranked based on the sum of size and weighted fitness. The individuals from the second list are presumably different in structure and fitness from the ones in the first list. The goal is to evolve solutions of minimal size that solve the problem. By directly using the size constraint the GP algorithm would be prevented from finding solutions. In contrast, the disassortative mating algorithm improves convergence to a better optimum while maintaining speed.

Two other diversity measures discussed in (Rosca, 1995) are the distribution of complexity of individuals (expanded structural complexity) and the distribution of fitness values. The latter is a more direct and easily observable type of variation in the population. Two individuals are different if they score differently.

Figures 1 and 2 present three dimensional plots with the fitness distributions for runs of GP and ADF-GP on the Even-5-Parity problem. These plots offer a compact representation of the fitness histograms used in (Koza, 1992). Koza pointed out that fitness histograms “give a highly informative view of the progress of the learning process for the populations a whole.” Note also that Figure 2, corresponding to GP with subroutines (in the ADF model) determines a much wider distribution of values for parity problems. The use of functions determines an increased exploration of the search space (Rosca, 1995) which positively affects the efficiency of GP.

Such information can be succinctly described using Shannon’s information entropy formula and represents a global measure for describing the state of the dynam-

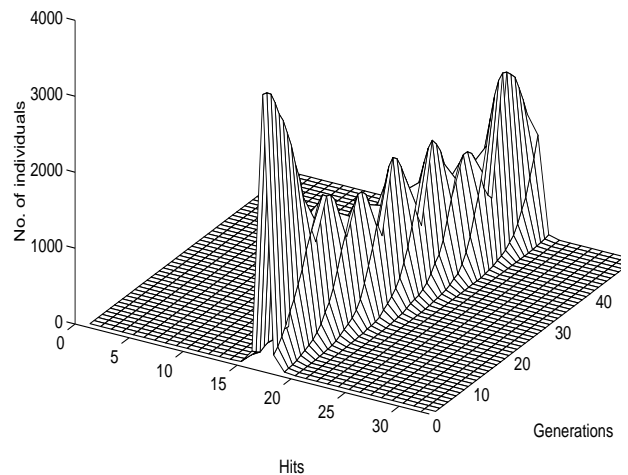


Figure 1: Fitness distributions over a run of GP on the Even-5-parity problem.

ical system represented by the population, in analogy to the state of a physical or informational system:

$$E(P) = - \sum_k p_k \cdot \log p_k$$

where p_k is the proportion of the population P occupied by population partition k at a given time.

Entropy has been used as a measure of diversity of an evolving ecological community in (Ray, 1993). Partitions were defined as individuals having the same genotype.

In a functional approach such as GP, an appropriate measure of diversity is obtained by grouping individuals in classes according to their behavior or phenotype and computing the population entropy based on the number of individuals belonging to each of these classes.

7 ENTROPY EXPERIMENTS

7.1 Experiments

This section examines the relation between diversity and fitness variation. Four examples are presented, from two problem domains: Boolean regression and controlling an agent in a dynamic environment (similar to the Pac-Man problem described in (Koza, 1992)). Each example discusses the relationships between the best-of-generation fitness, the average population fit-

ness (called energy in our earlier discussion) and diversity, as measured by the entropy formula. I used a population size of 4000, and ran the GP system for 50, and in several cases for 200, generations. Other GP parameters were chosen as in (Koza, 1994). The GP termination criterion did not take into account whether a solution was found.

The plots showed in this section represent three measures of interest: the best-of-generation individual (hits), the population average fitness (energy) and the population entropy. On each graph, numbered markers indicate the appearance of better best of generation individuals. The markers are also used to relate the fitness and entropy plots. The fitness and hits graphs (best-of-generation number of hits and average population fitness) have the value axis on the left while the entropy plots have the value axis on the right.

7.1.1 Even-5-Parity in standard GP

In this example better best-of-generation individuals appear very often in the first 30 generations (up to marker 1 in Figure 3). Thus, the system does not reach a stable state during this period. However, in generation 30, an apparition of a new best-of-generation individual is followed by a longer plateau of the hits plot at 23 hits. This plateau could be predicted by the variation in entropy, as entropy increases and then decreases between verticals marked 2 and 3. Figures 5 and 4 show the long term evolution in this run.

7.1.2 Even-5-Parity in AR-GP

In each of generation 1, 2 and 3 new functions were created based on useful building blocks (see figure 6). The new functions actually solve the parity problem on a subset of inputs. The system rapidly found a solution in generation 3 (32 hits). Soon after a solution was found (marker 1) a drop in value followed by a constant entropy value indicated a stable state. This was also reflected by the plateau in the average fitness and hit plots.

7.1.3 Even-5-Parity in ADF-GP

An example from a run of ADF-GP on the same problem is presented in Figure 7. After the sharp increases in the number of hits of the best-of-generation individual (markers 1, 2, 4, 5), the entropy increases for a short number of generations but then starts to decrease. This is very clear at marker 5. The discovery of a new best-of-generation individual is done after a period of relative stability (markers 4-5), indicated by the steady decrease in entropy. Note that, again, after marker 5 (generation 35), a new stable regime is reached.

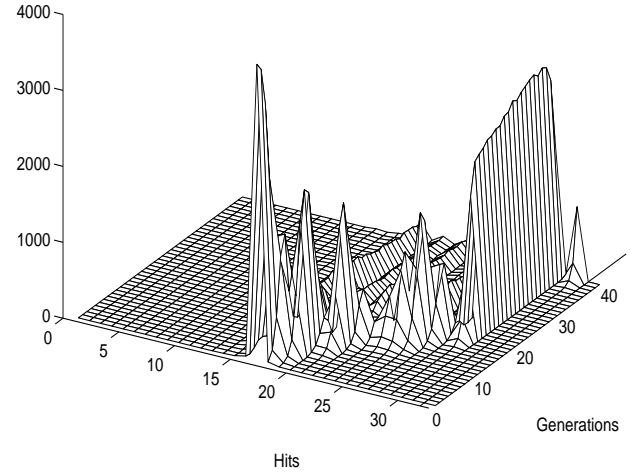


Figure 2: Fitness distributions over a run of ADF-GP on the Even-5-parity problem.

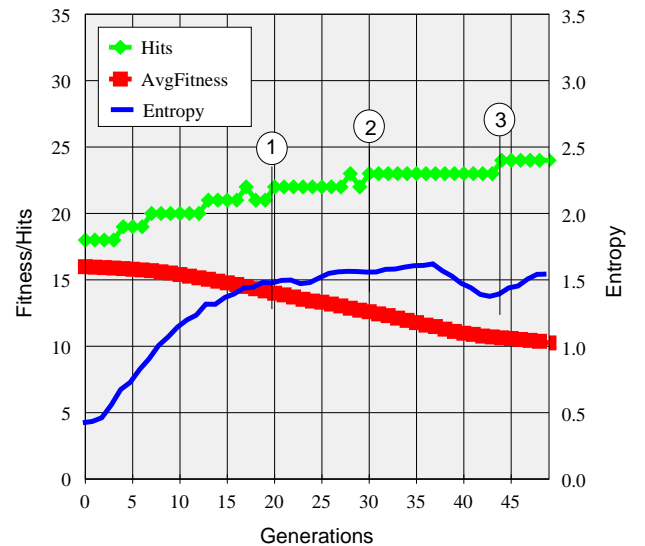


Figure 3: Entropy reflects population diversity and suggests local search optima. Marked points indicate sharp increases in fitness of the best-of-generation individual in two Even-5-Parity runs due to discovery of new functions. Entropy decreases are correlated with plateaus in fitness and indicate loss of population diversity and stable search regions (see also Figures 6, 7, 8).

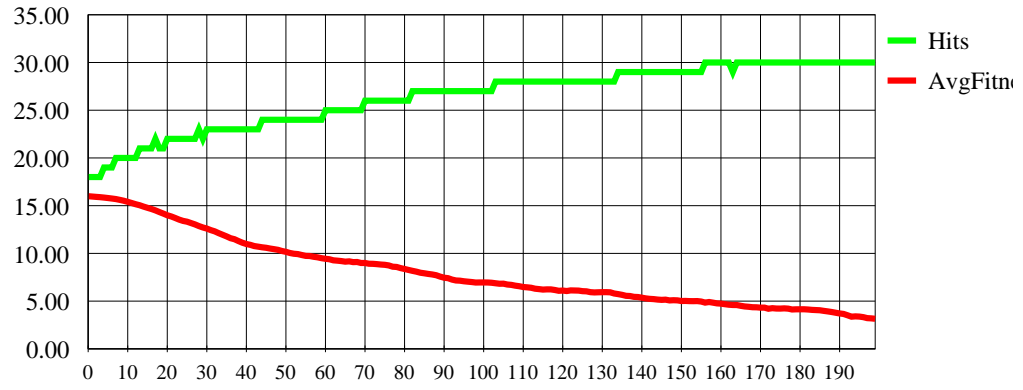


Figure 4: Best-of-generation number of hits and average fitness in a run of the parity example for 200 generations. The first part of this run is detailed in Figure 3.

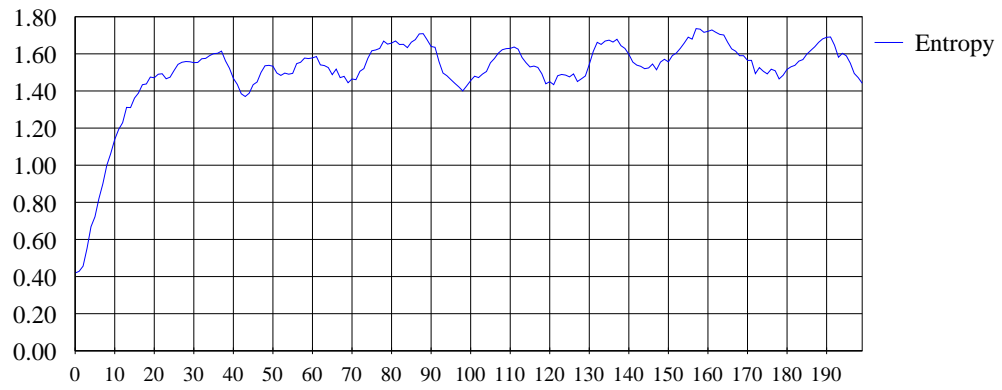


Figure 5: Entropy variation in the run of the Even-5-Parity example from Figure 4.

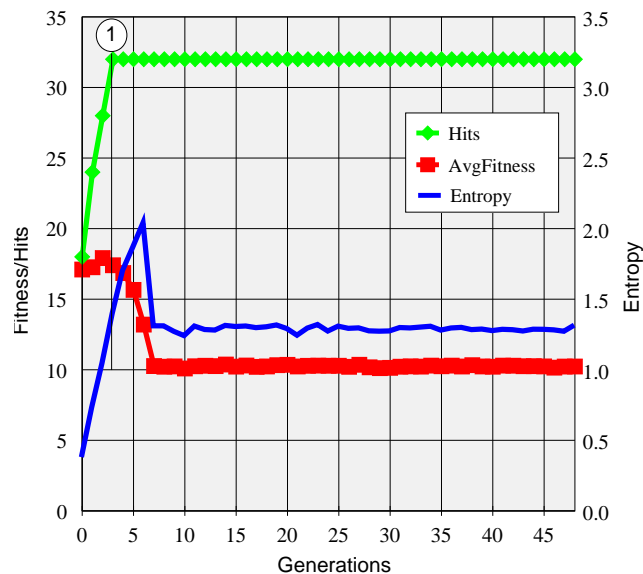


Figure 6: Fitness distributions over a run of AR-GP on the Even-5-parity problem.

7.1.4 GP on the Pac-Man problem

A run of GP on the Pac-Man problem is presented in figure 8. Each of the markers indicates periods of relative stability. This is more obvious on the intervals 4-5 and 5-on. Although the entropy has the general features from the previous examples, it is much more noisy. This can be due to the increased instability of solutions in the Pac-Man domain and to the very large distribution of solutions.

In order to filter out some of the noise, classes should have larger granularity. For instance, the total range of hits could be partitioned into a collection of intervals. All programs with the number of hits belonging to the same interval should be in the same class.

7.2 Discussion

The examples above present common patterns and suggest the following conclusions:

1. Plateaus or monotonic decreases in population entropy over an increased number of generations indicate possible local search optima. These are associated to plateaus on the best-of-generation individual hit plots.
2. Entropy decreases correspond to decreases in population diversity but not necessarily to decreases in fitness.

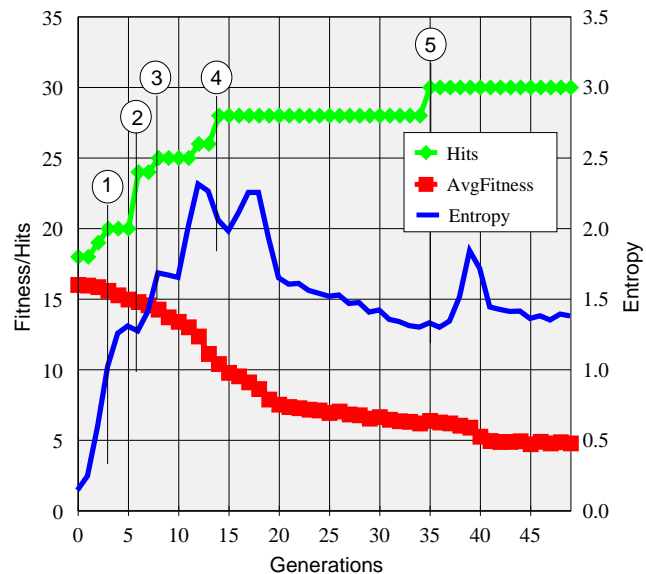


Figure 7: Fitness distributions over a run of ADF-GP on the Even-5-parity problem.

3. An improvement in average fitness may be caused by the selection of above average individuals in larger proportions and does not necessarily show that beneficial changes are made in the population composition. However, such a cause would generate effects in the fitness plots.
4. The correlation between entropy (i.e. population diversity) and energy (i.e. average fitness) suggests when computational effort is wasted due to local minima.

Goldberg discussed the tradeoff between precision, given by better optima, and computational effort, measured simply as running time, in GAs (Goldberg, 1989). He showed that new operators are used in order to maintain diversity in the population and that increased diversity causes decreased performance due to an increase in computational effort.

We suggest that this is not necessarily the case in GP. Computational effort should be spent so that diversity is increased only when there is clear evidence that search has reached a local minimum. A description of phenotypic diversity based the entropy formula appears to be useful when correlated with other statistical measures extracted from the population. Such a measure would also be computationally inexpensive.

One of the main goals of this work is to determine when creation or modification of functions is advantageous or necessary (the “when” problem mentioned previously). I suggest that entropy is a suitable measure for controlling the adaptation of the problem representation by creating new functions. While entropy

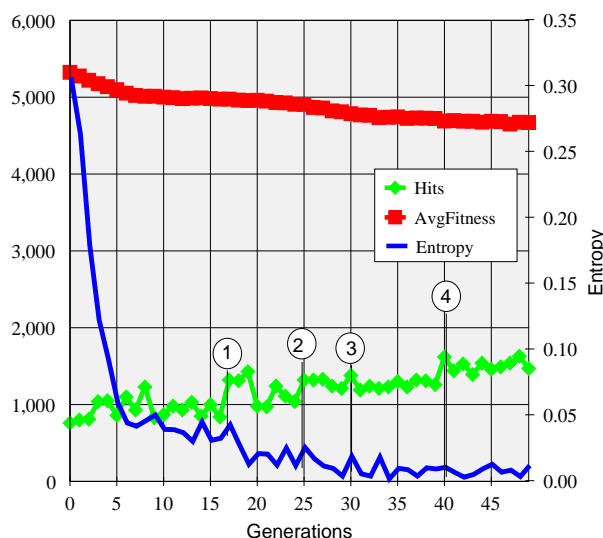


Figure 8: Fitness distributions over a run of GP on the Pac-Man problem.

is a good measure for tracking diversity, the discovery of new functions is the actual mechanism used for increasing diversity and escaping local optima (Rosca, 1995). The definition and use of new functions determines an exploration of the search space of programs.

8 CONCLUSIONS AND FUTURE WORK

Two main strategies are at work in GP: exploration and exploitation. In other search techniques, abstracted by the two-armed bandit problem, such as reinforcement learning (Whitehead, 1992; Kaelbling, 1993) one has explicit control over how much exploration and how much exploitation is performed. Control is tweaked also according to an explicit scheme in classifier systems. In the reinforcement phase of the control loop of a classifier system, matching classifiers that do not get activated are weakened. This lowers the chances of choosing unpromising actions in the near future. The weakening magnitude is usually controlled by an explicit parameter, although more elaborate schemes are possible (Wilson, 1994).

In GP one no longer has control over how much is exploitation and how much is exploration, because it is hard to delimit exploration from exploitation. This is one of the weaknesses of GA in general and GP in particular, but is also one of the advantages. This is a weakness because one prefers to search nice, smooth landscape surfaces. The GP representation does not define such a surface. Also, this is an advantage, because the crossover operator enables the exploration of

new regions of the space. However, in the case of GP with subroutines crossover has a substantial destructive effect. Adaptive techniques should ensure that GP does not waste its search effort.

GA research has suggested that although maintaining diversity leads to better optima, a cost has to be paid as computational effort increases. In contrast, I argue that in GP diversity can be correlated to other statistical measures, such as average population fitness, in order to intelligently control the exploration-exploitation tradeoff.

Two main directions of future work are theoretical analysis and experimental validation. An interesting idea from the former perspective is to correlate energy and entropy using the free energy concept. Free energy may show even clearer whether the system moves towards more improbable states and evolves. It may provide a statistical interpretation to the ripples of evolution.

Experiments based on an estimation of the computational effort will finally validate the hypothesis that entropy driven adaptation of the problem representation may prove economical after all. This remains a goal for the near future.

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