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Finding Building Blocks Through Eigenstructure Adaptation

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Abstract

A fundamental aspect of many evolutionary approaches to synthesis of complex systems is the need to compose atomic elements into useful higher-level building blocks. However, the ability of genetic algorithms to promote useful building blocks is based critically on genetic linkage – the assumption that functionally related alleles are also arranged compactly on the genome. In many practical problems, linkage is not known a priori or may change dynamically. Here we propose that the problems' Hessian matrix reveals this linkage, and that an eigenstructure analysis of the Hessian provides a transformation of the problem to a space where first-order genetic linkage is optimal. Genetic algorithms that dynamically transform the problem space can operate much more efficiently. We demonstrate the proposed approach on a real-valued adaptation of Kaufmann's NK landscapes.

Introduction

A fundamental aspect of many evolutionary approaches to synthesis of complex systems is the need to compose atomic elements into useful higher-level building blocks. This compositional process should continue recursively to generate increasingly complex modules from lower level components, until the desired solution is attained. The importance of discovery of partial building blocks was initially stresses by Holland (1975) in "The building block hypothesis" that described how Genetic Algorithms (GAs) work. GAs promote useful building blocks represented as schemata, and compose them though the process of crossover. As the Schema Theorem shows, however, the ability of GAs to promote useful building blocks is based critically on genetic linkage – the assumption that functionally related alleles are also arranged compactly on the genome. If genetic linkage is poor (i.e., there is little correlation between functional dependency and genetic proximity), then the crossover operator is more likely to break useful building blocks than it is likely to compose them.

The effect of poor genetic linkage can be dramatic. Before proceeding to describe previous work and our proposed solution, we demonstrate the grave effect of poor linkage in Figure 1. The graph shows the best population fitness of a GA running on a hard test problem. The test problem consists of 16 real-valued dimensions, each of which is deceptive (gradients lead in the wrong direction), and contains significant coupling between the variables. The test problem will be described in detail later; for now, it is suffice to notice the difference in performance of the GA between the top curve, where the genome is ordered so that coupled variables are close to each other (tight linkage), versus the lower curve, where the genome is shuffled so that coupled variables are far from each other (poor linkage). In both these cases, diversity maintenance techniques were also used. Without diversity maintenance, the GA's performance is inferior even to standard optimizers such as a well-tuned parallel simulated-annealing optimizer and a parallel random mutation hillclimber (a basic gradient optimizer). A random search process is shown for reference. All methods perform equal number of samplings per generation.

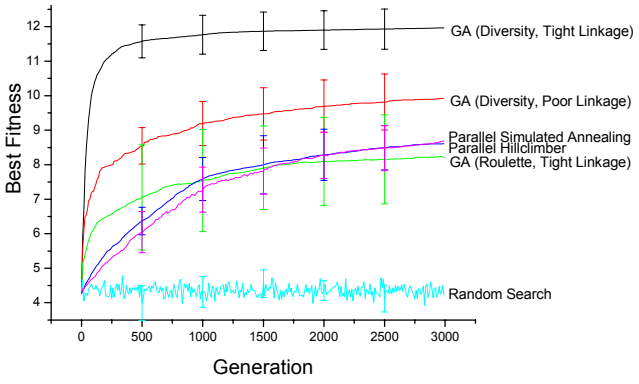

Figure 1. Performance of a GA on a 16 dimensional problem with poor and tight linkage, with and without diversity maintenance. A parallel Simulated Annealing optimizer, a parallel hillclimber, and a random search are provided for comparison. All methods perform equal number of evaluations per generation. Error bars of one standard deviation based on 10 runs on the same problem.

Since genetic linkage is not necessarily known in advance, and may change dynamically as solution progresses or as the problem varies, new evolutionary algorithms have been proposed that either change linkage dynamically, or that do not rely on genetic linkage at all (at an additional computational cost). Originally, Holland (1975) proposed an inversion operator that would reorder alleles on the genome, with the expectation that genomes with better

orderings (tighter genetic linkage) would gradually take over the population. However, this operator turned out to be too slow in practice. A variety of algorithms were proposed that do not assume linkage at all, and build up the genome from scratch starting with the founding building blocks. Goldberg *et al* (1989) developed the *Messy GA* that evolves partial solutions in which allele locations are moveable, and linkage can be adapted through combination and split operators. Genetic programming (Koza, 1989) combines building blocks in tree hierarchies, allowing arbitrary branches of solutions to be swapped and thereby permitting promotion of useful subcomponents without relying on linkage (although GP is usually applied to open-ended problems where linkage is not well defined anyway). More recently, Harik and Goldberg (1996) proposed a linkage learning genetic algorithm (LLGA) that intersperses alleles in the partial solutions with variable-sized gaps (*introns*) allowing the GA more control over linkage tightening and exchange of complete building blocks. A more recent version of this algorithm uses evolved start expressions to assist in the process of nucleation of tightly linked groups (Chen and Goldberg, 2002). Watson and Pollack (2002) also co-evolve partial solutions, but use symbiotic completion and Pareto-dominance criteria to compare candidate subcomponents, and assemble full solutions from scratch without assuming linkage. The increased computational cost comes through the exploration of many compositional permutations offered by this formulation, but both of these approaches have been shown to be able to synthesize solutions to complex functions with multiple local optima, which traditional GAs and gradient optimizers cannot solve.

Identifying linkage through the Hessian

Here we propose an alternative way of identifying building blocks through dynamic eigenstructure analysis of the problem landscape's Hessian matrix. The matrix H is defined by measuring the cross-correlation effect of the variation of each of the n variables x_i on the variation effect of each other locus of the genome on the fitness function $F(X)$. Essentially, the Hessian matrix determines the first-order functional dependencies between gene locations. The Hessian is defined as

$$H_{ij} = \frac{\partial F(X)^2}{\partial x_i \partial x_j} \tag{1}$$

By definition, it is a symmetric matrix. For example, if

$$X=(x_1, x_2, x_3, x_4), \tag{2}$$

and the fitness function to be optimized is

$$F(X)=\sin(2x_1x_3)+\sin(3x_2x_4), \tag{3}$$

then computing H and evaluating at X=0 would yield

$$H = \begin{bmatrix} 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \\ 2 & 0 & 0 & 0 \\ 0 & 3 & 0 & 0 \end{bmatrix} \tag{4}$$

Highly coupled variable pairs are represented by large magnitude elements in H. Large, off-diagonal elements imply coupling between variables that are not adjacent on the genome; to improve linkage, variables can be rearranged so that coupled pairs are proximate on the genome, bringing their corresponding Hessian coefficient closer to the diagonal. Rearranging the order of parameters is equivalent to swapping rows and columns of H, effectively transforming by a permutation transformation. To bring the elements of H above closer to the diagonal (effectively tightening the genetic linkage), we can use the permutation matrix T, where

$$T = \begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \tag{5}$$

to yield a new Hessian H',

$$H' = T^T H T = \begin{bmatrix} 0 & 2 & 0 & 0 \\ 2 & 0 & 0 & 0 \\ 0 & 0 & 0 & 3 \\ 0 & 0 & 3 & 0 \end{bmatrix} \tag{6}$$

and the improved genome ordering X'

$$X' = XT = \{x_3, x_1, x_2, x_4\} \tag{7}$$

H' above is as close as we can bring the non-zero elements to the diagonal by reordering, and the resulting genome ordering of Eq. (7) has indeed improved its linkage compared to the original ordering of Eq. (2). But is there a way to bring them even closer to the diagonal?

Generalized genome reordering

The optimal linkage ordering is not necessarily sequential. In the example above, the permutation matrix simply reorders elements on the genome. However, there might not be a perfect sequential ordering if variables are coupled in any way but a linear serial chain. For example, if three variables are coupled equally, there is no way to arrange them in linear progression so that all are equally close to each other (the first will be less proximate to the last than it is to the middle variable). Similarly, in the previous example of Eq. (3), x_1 is coupled to x_3 but not to x_2, so the genome ordering provided in Eq. (7) is still not optimally tight, and that is why H' is not exactly diagonal.

However, since the permutation matrix is nothing but an orthogonal linear transformation, we can think of any reordering process as merely a linear transformation. Now, by allowing the transformation to have non-integer elements, we can allow for even more compact orderings. Essentially, the optimal transformation is the one that will bring all elements of the Hessian matrix *exactly* to the diagonal. We thus seek the optimal transformation T_0 to a diagonal matrix λ:

$$T_0^T H T_0 = \lambda \tag{8}$$

Solving for T_0 yields the Hessians' eigenvectors[1]. Because the Hessian matrix is always symmetric, the eigenvectors have no imaginary component. In our example,

$$T_0 = \frac{\sqrt{2}}{2}\begin{bmatrix} 0 & -1 & -1 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & -1 & 0 \\ -1 & 0 & 0 & 1 \end{bmatrix} \tag{9}$$

and

$$H_0 = T^T H T = \begin{bmatrix} -3 & 0 & 0 & 0 \\ 0 & -2 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 3 \end{bmatrix} \tag{10}$$

and the optimal genome ordering X_0 is given by

$$X_0 = XT_0 = \frac{\sqrt{2}}{2}\{< x_2, -x_4 >, < x_3, -x_1 >, \\ < -x_1, -x_3 >, < x_2, -x_4 >\} \tag{11}$$

To understand why the linkage-optimal vector X_0 above has even less coupling than the compactly ordered vector $X'=\{x_3, x_1, x_2, x_4\}$ of Eq, (7), consider the following. A small positive mutation δ applied to x_1, a gene of X', will result in either an increase or decrease of the fitness function. Whether it will be an increase or a decrease depends on the sign of another gene, x_3, thus there is still coupling between alleles on the genome. On the other hand, a small positive mutation in δ applied to $<x_1,x_3>$ will always result in an increase in fitness, regardless of the states of other genes. Therefore, $<x_1,x_3>$ is more suited to be a gene than any single variable. Similarly, a small positive mutation δ applied to the complementary vector $<x_1,-x_3>$, the second gene of X_0, will do nothing to the fitness function, independent of the value of the other variables. These two thus genes span the search space much more effectively.

[1] Assuming $H \neq 0$. If H is null, the landscape is linear or constant and no linkage problem exists.

What can we learn from the eigenvalues?

The eigenvalues λ hold the scaling factors of the new space, by which any variation operators can be calibrated; in our example, these are 2 and 3. Dividing the mutation operators, for example, by these factors would allow all blocks to be explored at the same resolution.

Degenerate eigenvalues (two or more eigenvalues of the same magnitude) indicate a subspace of the landscape, spanned by the corresponding eigenvectors, where variables are uniformly coupled (or decoupled). For example, the fitness function of Eq. (3) has two degenerate sets, implying two such subspaces, the subspace spanned by x_1 and x_3 and the subspace spanned by x_2 and x_4. In a degenerate subspace the eigenvectors are not unique.

Using transformations in a GA

Based on the analysis above, we conclude that

- The genome reordering is equivalent to a linear transformation of the fitness landscape, therefore,
- There exists non-discrete genome orderings, and
- The ordering that yields optimal genetic linkage at a point in the landscape is given by the eigenvectors of the Hessian at that point.

Once a linkage-optimal ordering transformation has been determined by computing the eigenvectors of the Hessian of $F(X)$, a GA can proceed regularly by evolving individuals h_i, but evaluating $F(T_0 h_i)$, instead of directly $F(h_i)$. Many varieties of GAs, such as those incorporating partial solutions, learning, and sophisticated composition operators can easily be modified to use this formulation.

Test function

We tested the eigenvector reordering process on evolution of a solution to a multidimensional function of real variables, $Z(X)$, that composes n base functions $\Psi(x)$:

$$Z(X) = \frac{1}{2}\sum_{i=1}^{n} \Psi(b_i) \tag{12}$$

where

$$\Psi(u) = \frac{\cos(u)+1}{|u|+1} \qquad b_i = \sum_{j=1}^{k} a_{ij} x_{(i+j) \bmod n} - c_i \tag{13}$$

This function is a real-valued adaptation of Kauffman's NK landscapes (1993). Kauffman defined a function with N bits, in which each bit's fitness contribution depends arbitrarily on its K neighbors. NK landscapes thus have "tunable ruggedness" and are often used to test GAs. Here

we defined a similar problem that uses real values instead of bits. First, we define a multimodal base function $\Psi(x)$ with one global maximum at c_i, and several smaller maxima, shown in Figure 2. The constants c_i are each set arbitrarily. This base function is deceptive if the search space is larger than $\pm 2\pi$ around c_i, because then in most of the space the gradients lead to local optima. The function Z is a sum of the n single dimensional base functions; however the blocks are not separable: Each base function is evaluated at position bi, which is a mixing function of k elements of the argument vector X. The mixing is obtained through an array of coefficients a_{ij}, each set arbitrarily. Because of the mixing of order k, optimizing one dimension may (and usually does) lead to adverse effect in the other k-1 dimensions. Finally, the genome elements $x_{i..n}$ are shuffled so that variables that contribute to the same base function are maximally apart on the genome, so as to create the worst linkage. The function was defined so that it always has a single global optimum with the value n, and it occurs at $X=A^{-1}c$ (where A is a k-diagonal matrix with the elements of a on its diagonals, and X is the unshuffled vector). In our study, we generate the coefficients a_{ij} randomly with a uniform distribution in the range of ± 1, and the coefficients c_i with a uniform distribution in the range of ± 8. These values were selected arbitrarily, and were not tuned.

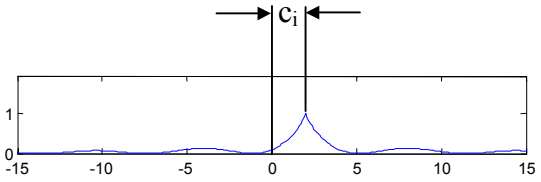

Figure 2. The base function $\Psi(x)$ used to construct the test function. The full test function is a shuffled k^{th}-order mixing of n base functions.

Experimental Results

We carried out a series of tests, with different setting of N and K. All problems have bad shuffling (poor linkage). In each experiment, we set the coefficients randomly, and then carried out several runs to collect average performance and standard deviation. We also ran a parallel hillclimber as a baseline control.

In all experiments we used a GA with a diversity maintenance technique called 'Deterministic Crowding' (Mahfoud, 1996). Diversity maintenance is important to avoid premature convergence, in which case crossover operators would do little and the effect we wish to study would vanish.

First, let us look closely at the effect of using a Hessian Eigenvector transformation. Figure 3 shows average performance of an Eigenvector GA on a problem with N=16 and K=4, for the first 500 generations. Population size is 100, and statistics are based on 20 runs. The transformation is re-computed numerically every 100 generations, around the currently best solution, adding 1% evaluations. We will discuss the cost of this computation in the next section. The points of re-computation are marked with a vertical dashed line; note how the process 'boosts' its optimization rate at those intervals.

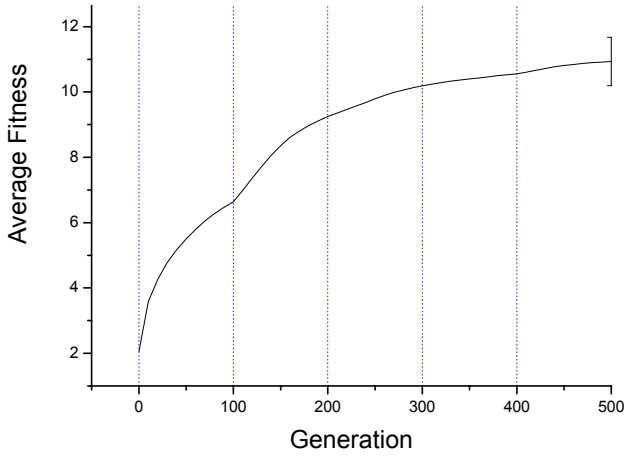

Figure 3. Performance of a GA on a shuffled real-valued NK landscape with N=16 and K=4. Reordering transformation is recomputed every 100 generations (at vertical dashed lines), and performance boosts are visible at those instances. Statistics are of 20 runs. Eigenvector GA uses 1% more evaluations.

Figure 4 shows the long-term behavior of the solver over 3000 generations using the same parameter settings. Both average fitness of the population and best fitness in the population are shown. We see that the eigenvector GA has significantly outperformed the regular GA. The contribution of the eigentransformation has been exhausted after 500 generations or so. After that period, both algorithms progress at roughly the same rate. We hypothesize this point is where contribution of first-order (linear) linkage has been exhausted. All runs use the 'deterministic crowding' diversity maintenance technique (Mahfoud, 1995).

The performance boost provided by the eigentransformation becomes more significant as the problem becomes harder both in the number of parameters (N) and in the amount of coupling between the parameters (K). Figure 5 shows the performance of an Eigenvector GA on a problem with N=64 and K=8. Population size is 100, and average and standard deviation is based on 10 runs. At N=256 and K=16, and at N=1024 and K=32, we observed similar performance boosts.

Computational Cost

While we understand why and how the eigenstructure can resolve linkage, we still need to determine when in generational time and where in the landscape to compute it. The cost associated with our method is composed of two independent factors: Arithmetic cost, and evaluation cost.

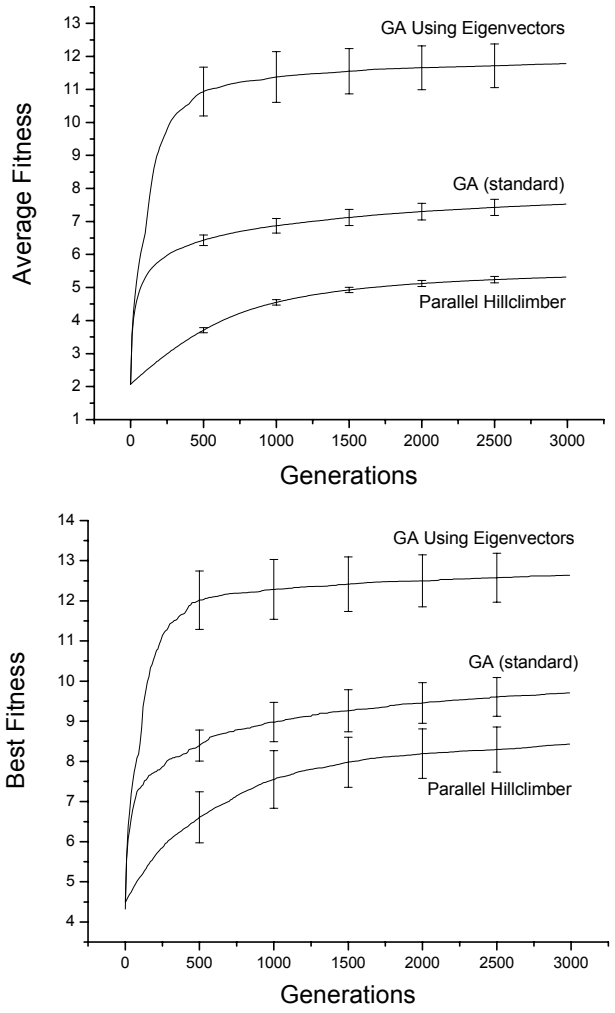

Figure 4. Performance comparison on a shuffled real-valued NK landscape with N=16 and K=4. Reordering transformation is recomputed every 100 generations. Statistics are of 20 runs.

The evaluation cost has to do with the increased number of evaluations needed to compute the Hessian. The arithmetic cost is the added computation associated with analyzing and using the Hessian. We discuss both costs here.

Arithmetic cost

Additional computational cost is incurred by the linear transformation and eigenstructure calculation. The transformation cost adds $O(n^2)$ arithmetic operations per evaluation and $O(n^2)$ arithmetic operations per Hessian calculation for computing derivatives from the samples, and computing the eigenvectors. Both of these are typically negligible compared to the cost of a single evaluation of hard practical problem.

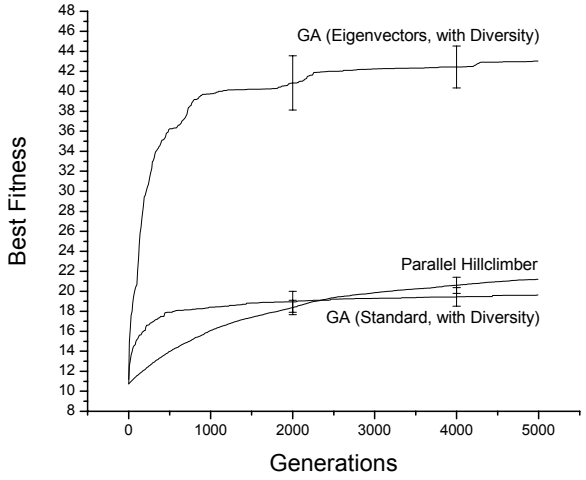

Figure 5. Performance comparison on a shuffled real-valued NK landscape with N=64 and K=8. Reordering transformation is recomputed every 200 generations. Statistics are of 10 runs.

Evaluation cost

The evaluation cost is especially critical because direct numerical calculation of the Hessian matrix involves approximately $2n^2$ samplings of the search space. If each individual is at a different location of the landscape, this may amount to $2n^2p$ extra evaluations per generation, where p is the population size. This cost is prohibitive, and so more efficient schemes must be found.

If linkage properties of the landscape are *consistent over time*, significantly fewer than n^2p samplings are necessary. For example, the results shown in Figure 4 required only one Hessian calculation per 100 generation. Since for that problem $n=16$, this amounts to only 1% additional evaluations, and the advantage gained is well worth it. The number of evaluations grows as $O(n^2)$ but the interval at which Hessian-recalculation is required increases as well since propagation of building blocks is slower.

If the linkage properties of the landscape are *consistent over space*, the Hessian does not need to be tracked for every individual. For the results shown in Figure 4 we recalculated the Hessian only around the currently best individual, but use it for all individuals in the diverse population.

It is conceivable that a harder class of problems exists where *linkage properties* of the landscape change over time and over space. Prior work dealing with various forms of linkage learning and composition has typically assumed the linkage properties are fixed for the given problem. For such linkage-variable problems we might either spend more evaluations to track separate Hessian matrices for clusters of individuals, and also update them more frequently. Alternatively, we could extract Hessian information indirectly from the samplings already being done by the GA anyway.

Indirect computation of the Hessian

The Hessian can be computed indirectly from the GA samples using cross-correlation statistics. As described by the "Two-armed Bandit" problem (De Jong, 1975), there is a tradeoff between *exploration* and *exploitation*. Some samples of the search space can be used to learn properties of the landscape (exploration), while other samples are used to maximize the fitness function at promising areas (exploitation). However, with a linkage-learning algorithm as proposed here, it is possible to use all samples to extract linkage properties and thus enhance exploration without incurring additional function evaluations, assuming linkage properties are persistent.

The key to indirect extraction of linkage information is the understanding that linkage can be learned just as efficiently even from individuals with low fitness. Consider, for example, a new individual in the population that is generated through crossover and yields a low fitness. In a traditional GA, this new individual is likely to be removed from the population. The information gained by that experiment is mostly lost: Although the frequency of the genes that made up that new composition has gone down, there was no recording of the bad functionality correlation that has been exposed by that composition. A linkage-learning algorithm, however, uses this information. Even when a new individual has low fitness, its fitness exposes important linkage properties that are critical to efficient composition of new, more successful individuals in the future.

Estimating the Hessian through least squares

One way to gather linkage properties from arbitrary, unstructured samplings of the search space is through least-squares fitting to a linkage modeling function. For example, assume a two dimensional landscape $F(x_1,x_2)$ can be described very roughly by the conic section equation

$$F(x_1, x_2) = ax_1^2 + 2bx_1x_2 + cx_2^2 + dx_1 + ex_2 + f \quad (12)$$

The linkage coefficient we are interested in is the magnitude of parameter *b* with respect to parameters *a* and *c*. These parameters reveal how the landscape is influenced by the combination (x_1x_2). Note that the function is not used to model the landscape for direct optimization; that is, we do not proceed to compute the optimum of *F*, because there is no guarantee whatsoever that the landscape is of degree 2 (in fact, if it was then much more efficient optimization techniques could be used). Instead, we only use it to probe how variables are dependent on each other, by fitting a conic surface to a small patch of the landscape. A landscape with *n* parameters will have $(n+1)(n+2)/2$ coefficients, and so $O(n^2)$ samplings will be needed to determine the coefficients through least squares modeling. Direct computation of the Hessian also requires $O(n^2)$ samplings, and so the new formulation is not a improvement in terms of the number of evaluations. However, the direct computation method required structured samplings on a grid, whereas the new formulation can use an unstructured pattern of samples, and can therefore use samples performed anyway by the GA in course of its normal operation.

The quality of the 'linkage probe' degrades as the sampling radius δ increases, just like direct numerical computation of the Hessian degrades with $O(\delta^2)$ according to Taylor expansion around the center point ($\delta \approx 0.1$ for the test function described in this paper). It is therefore necessary to use samples that are within small region with respect to nonlinearities in the function. In a diverse set of samples this can be done by clustering samples into groups, at the cost of additional cluster management.

Higher-level compositions

Direct eigenstructure transformation resolves first order linkage, but more elaborate, non-linear transformations may resolve higher order linkage. We say a linkage is first order when the linkage between two variables does not depend on any other, third variable. If it does, we would have a second order linkage. Higher order linkage effects can be identified using Kronecker tensor products of partial derivatives of arbitrary orders. High eigenvalues of these tensors indicates a strong high-order dependency that can be resolved through a nonlinear transformation. These higher order transformations are again provided by (nonlinear) eigenstructure analysis of tensors (Lipson and Siegelmann, 2000). In many ways, the approach proposed here is akin to support vector machine (SVM) methods (Cristianini and Shawe-Taylor, 2000) that transform the space so that data classes are linearly separable. Here, we use kernels (polynomial or other) that transform the search space so that linkage is optimal (linear).

Conclusions

Performance of genetic algorithms is critically based on both diversity maintenance and genetic linkage. Here we propose that linear transformations can effectively be used to reorder the genome, and that the linkage-optimal transformation can be found through Eigenstructure analysis of the landscape's Hessian matrix. In a series of experiments using a highly coupled, nonlinear, deceptive and shuffled function, we show how the presented algorithm produces significantly superior performance, at relatively low additional computational cost.

We also postulate that a new class of problems exists which is harder for GAs. These are problems where linkage properties of the landscape change over time and across the landscape. We define these problems as having high-order linkage. For such problems, linkage can be measured dynamically using statistical probes that use

existing evaluations. We further suggest that kernel methods that are traditionally used in machine learning to transform coupled problems into linearly separable problems, can be brought to bear on evolutionary computation to decompose high-order linkage into linkage optimal.

Acknowledgments

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