Gene Expression and Fast Construction of Distributed Evolutionary Representation

Hillol Kargupta

School of EECS Washington State University Pullman, WA 99164-2752, USA hillol@eecs.wsu.edu Byung-Hoon Park

School of EECS Washington State University Pullman, WA 99164-2752, USA bhpark@eecs.wsu.edu

Abstract

The gene expression process in nature produces different proteins in different cells from different portions of the DNA. Since proteins control almost every important activity in a living organism, at an abstract level gene expression can be viewed as a process that evaluates the merit or "fitness" of the DNA. This distributed evaluation of the DNA would not be possible without a decomposed representation of the fitness function defined over the DNAs. This paper argues that unless the living body was provided with such a representation, we have every reason to believe that it must have an efficient mechanism to construct this distributed representation. This paper demonstrates polynomial-time computability of such representation by proposing a class of efficient algorithms. The main contribution of this paper is two-fold. On the algorithmic side it offers a way to scale up evolutionary search by detecting the underlying structure of the search space. On the biological side, it proves that the distributed representation of the evolutionary fitness function in gene expression can be computed in polynomial-time. It advances our understanding about the representation construction in gene expression from the perspective of computing. It also presents experimental results supporting the theoretical performance of the proposed algorithms.

Keywords

Gene expression, representation construction, Walsh analysis, linkage learning.

1 Introduction

The last fifty years of this century witnessed the gradual development of different adaptive search algorithms that use motivations from natural evolution. The Genetic algorithms (GAs) [27], evolutionstrategie (ES) [62], evolutionary programming (EPs) [13], and genetic programming (GPs) [47] are some examples that found many successful applications in search, optimization, and machine learning. These algorithms are primarily motivated by the passage of evolutionary information from generation to generation through selection, crossover, and mutation operations. Evaluation of fitness in GAs, ES, EPs, and GPs is often a simple one step process of computing the objective function (with some exceptions [67]). However, this is not quite that simple in nature. This process (often called the gene expression) can be arguably viewed as a process that significantly contributes towards evaluating the evolutionary fitness of a genome through a sequence of representation transformations (DNA \rightarrow mRNA \rightarrow Protein). This paper questions the simplistic and centralized one-step event of the objective function evaluation often adopted in the practice of evolutionary algorithms. It draws atten-

tion to the gene expression process and argues that this complex process may have a non-trivial role in controlling the efficiency of the evolutionary search.

Although, today we have reasonable idea about the main biological steps of gene expression, we know very little about its role in evolutionary search. This paper takes a modest step in unraveling this mystery. It explores the computability of the decomposed representation of the evolutionary fitness function exploited during gene expression in the light of our existing understanding about inductive construction of function structure. It is not a paper on GAs or GPs or any other popular paradigm of evolutionary algorithms. However, it may have important implication in the future of evolutionary computation.

Gene expression involves construction of proteins from the DNA sequence. Since proteins play an important role in almost every major activity of a living body, the efficacy of the produced proteins determines its overall "fitness". So at a very abstract level gene expression can be viewed as a process that evaluates the evolutionary fitness. Interestingly enough, it does so in a very distributed fashion. Different portions of the DNA, the evolutionary information carrier, are evaluated in different cells through the production of different proteins. This paper suggests that the distributed evaluation of evolutionary fitness may have deeper implications. Distributed evaluation is possible only when the underlying fitness function can be represented in a decomposed form. Such representations also expose the underlying decomposability of the fitness function and therefore it is important for the scalability of any search algorithm, including evolutionary search [40]. Therefore, one must wonder if the gene expression process has a hidden mechanism to construct such representations. However, we must address a more fundamental question before exploring that intriguing possibility. We should first show that such a construction is feasible using our basic understanding of computation. This paper shows that this is indeed possible in polynomial-time when the number of mutually interacting genes is bounded regardless of the length of the genome.

Section 2 discusses the role of function induction in learning, adaptation, and optimization. Section 3 discusses the distributed fitness evaluation in the natural gene expression process and argues the need for an efficient function induction mechanism in our model of evolutionary computation. Section 4 discusses the previous work in evolutionary computation that considered gene expression. Section 5 briefly overviews the basics of orthonormal basis representation. Section 6 presents two algorithms to compute a distributed representation using orthonormal basis in polynomial time. Section 7 discusses the application of the proposed algorithms in detecting the search space structure. Section 8 presents experimental results of applying this algorithm to detect the underlying structure of different, difficult optimization problems. Section 9 discusses the future and on-going work and Section 10 concludes this paper.

2 Function Induction in Learning, Adaptation, and Optimization

Function induction plays an important role in machine learning, adaptation, and non-enumerative black-box optimization. In function induction the goal is to learn a function $\hat{f}: X^n \to Y$ from the data set $\Omega = \{(\mathbf{x}_{(1)}, \mathbf{y}_{(1)}), (\mathbf{x}_{(2)}, \mathbf{y}_{(2)}), \cdots (\mathbf{x}_{(k)}, \mathbf{y}_{(k)})\}$ generated by some underlying function $f: X^n \to Y$, such that \hat{f} approximates f. Any member of the domain $\mathbf{x} = x_1, x_2, \cdots x_\ell$ is an ℓ -tuple and x_j -s correspond to individual feature variables of the domain. Learning a function in a chosen form or representation is relevant to many important problem domains.

Empirical machine learning [52] is directly related to function induction. Given a

set of observed behaviors, the goal of empirical machine learning is to learn a function that closely approximates those behaviors, which is essentially the function induction problem itself when the behavior is viewed as a function defined over the domain of different situations.

Function induction also plays an important role in natural and artificial adaptation. The word adaptation literally means "to fit to" (ad + aptare). In general we call a system adaptive when it can exhibit appropriate behavioral dynamics in response to changes in an uncertain environment. Inductive function learning has a close relation with adaptation [27]. Adaptation in uncertain environments typically requires learning probabilistic behavior, learning to predict uncertain future, learning strategies to outsmart competitors, learning to co-operate, and others. All these learning problems typically involve empirical function induction from observed data.

Optimization in the absence of sufficient prior domain knowledge to guide search directions is often called black-box optimization (BBO). Typical BBO algorithms like evolutionary algorithms [27], simulated annealing [46] sample the search space and make inductive decisions in order to explore the promising parts of the search space. The optimization algorithms need to guess intelligently about the landscape using the samples taken from the search domain. This requires inductive detection of function structure.

Learning a function from data is indeed a common problem in many other domains like data mining, software engineering, pattern recognition, signal processing. Like all these problem domains, the emergence of adaptive living organisms through evolutionary search critically depends on function induction. Natural evolution can be viewed as a search for evolving systems that can adapt and survive the competition of natural selection. If this perspective is correct then the living organisms must have an efficient mechanism to learn functions from observed data. Indeed, there exist many facts that corroborate this observation. The role of neural networks in our brain is now widely recognized to be an important mechanism for learning functions from observed data [65]. This paper suggests that there may be an alternate mechanism for inducing function structure in the evolutionary operators of living organisms. The following section argues this possibility.

3 Fitness Evaluation Through Gene Expression

In nature the evaluation of the "fitness" of an organism is believed to take place through the expression of the DNA through the construction of proteins. This paper suggests that this process can be viewed from the perspective of function induction. It further advances the line of thought by pointing out that the construction of the representation of the genetic fitness may reveal a unique approach for inducing function structures from observed data. In order to fully appreciate this we need to understand the biology to some extent. The following discussion presents a brief exposure to the natural gene expression process.

DNA is the primary carrier of the evolutionary information that is transmitted from one generation to another. DNA molecules consist of two long complementary chains held together by base pairs. DNA consists of four kinds of bases joined to a sugar-phosphate backbone. The four bases in DNA are adenine (A), guanine (G), thymine (T) and cytosine (C). Chromosomes are made of DNA double helices. Bases in DNA helices obey the complementary base pairing rule. T and G pair with A and C respectively. In other words, if the base at a particular position of a helix is T then the corresponding base in the other helix should be A.

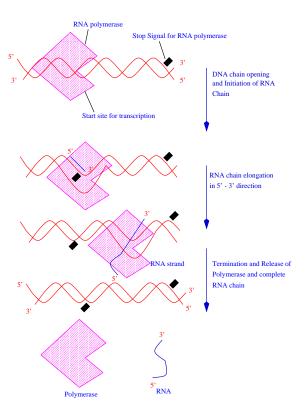


Figure 1: Transcription.

Evaluation of the fitness of a DNA takes place through a process called gene expression. Expression of genetic information coded in DNA involves construction of the mRNA sequence, followed by that of proteins. The main steps are,

- transcription: formation of mRNA (messenger ribonucleic acid) from DNA
- translation: formation of protein from mRNA
- protein folding

In a particular cell, transcription produces the mRNA from a small portion of the DNA. The mRNA defines another level of representation of the genetic information. It consists of four types of bases joined to a ribose-sugar-phosphodiester backbone. The four bases are adenine (A), uracil (U), guanine (G), and cytosine (C). All the bases defining the mRNA are same as those in DNA sequences, except that T is replaced by U. As shown in Figure 1, the mRNA is produced from the DNA by RNA Polymerase and the regulatory proteins following the complementary base-pairing rules similar to those in DNA. The RNA Polymerase initiates the transcription at a place of the DNA marked by the promoter region (start site). It splits the DNA double helix and continue generating the mRNA using one of the DNA strands as a template. The RNA Polymerase stops when it finds a termination signal sequence (stop site) in the DNA strand. Note that

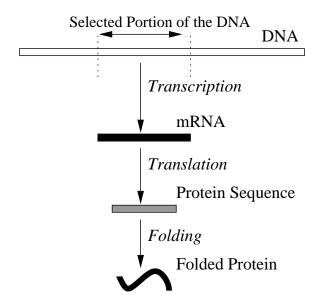


Figure 2: Different steps of gene expression.

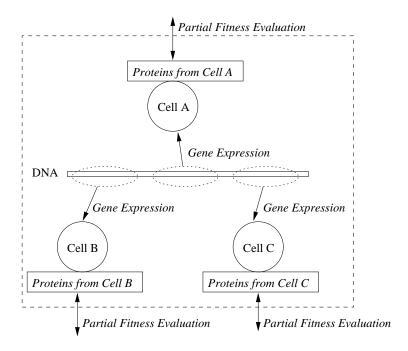
only a small portion of the DNA strand is transcribed and different cells may transcribe different regions of the DNA for producing proteins. Figure 1 presents a schematic diagram of the transcription process.

The mRNA acts as the template for protein synthesis. A protein is defined by a sequence of *amino acids*, joined by peptide bonds. The mRNA is transported to the cell cytoplasm for producing protein in the ribosome. There exists a unique set of rules that defines the correspondence between nucleotide triplets (known as codons) and the amino acids in proteins. This is known as the *genetic code*. Each codon is comprised of three adjacent nucleotides in a DNA chain and it produces a unique amino acid. Amino acid sequence defines a new representation of the information coded in mRNA.

The next level of representation of genetic information is defined by the three dimensional structure of folded proteins. Although amino acid sequences fundamentally define proteins, formation of the three dimensional structure of proteins involves a complex process, often called *protein folding*. This process involves interaction between multiple amino acid subsequences. Figure 2 shows the different steps of the gene expression process.

Since proteins control almost every important activity in a living organism, at an abstract level gene expression can be viewed as a process that evaluates the merit or "fitness" of the DNA. Since different proteins are generated at different cells from different portions of the DNA, fitness evaluation in natural gene expression appears to take place in a distributed fashion. In other words, the fitness evaluation seems to be decomposed into different sub-function evaluations. Figure 3 illustrates this distributed, decomposed evaluation of the evolutionary fitness. Such distributed fitness evaluation is possible under either of the two following conditions:

1. the distributed representation of the fitness function was available to evolutionary



ENVIRONMENT

Figure 3: Distributed, decomposed evaluation of the evolutionary fitness through construction of different proteins in different cells.

mechanism a priori;

2. the distributed representation of the function is inductively constructed from the sample DNAs and their respective fitnesses, observed in nature.

In the following sections we shall adopt the latter possibility and explore it in the context of our basic understanding about function induction. However, first let us review the existing literature in evolutionary computation that considers the computational role of gene expression.

4 Gene Expression in Existing Models of Evolutionary Computation

Although today gene expression is not emphasized very much in most of the popular models of evolutionary computation, several researchers realized its importance. The importance of the computational role of gene expression was realized by Holland. He described [27] the dominance operator as a possible way to model the effect of gene expression in diploid chromosomes. He also noted the importance of the process of protein synthesis from DNA in the computational model of evolution. Despite the fact that, traditionally, dominance maps are explained from the Mendelian perspective, Holland made an interesting leap by connecting it to the synthesis of protein by gene signals, which today is universally recognized as gene expression. He realized the relation

between the dominance operator with the "operon" model of the functioning of the chromosome [30] in evolution and pointed out the possible computational role of gene signaling in evolution [27].

Several other efforts have been made to model some aspects of gene expression. Diploidy and dominance have also been used elsewhere [2, 10, 28, 64, 69]. Most of them took their inspiration from the Mendelian view of genetics. The under-specification and over-specification decoding operator of messy GA has been viewed as a mechanism similar to gene signaling [23]. The structured genetic algorithm [11] also shares motivations from the gene expression; it uses a structured hierarchical representation in which genes are collectively switched on and off. This provides the search algorithm with a richer representation and helps capturing properties of the landscape better. Kauffman [42] offered an interesting perspective of the natural evolution that realizes the importance for gene expression. However, Kauffman's work does not explain the process in basic computational terms on analytical grounds and does not relate the issue to the complexity of search process. The "neutral network" theory [63] considers sequence-to-structure mapping from the perspective of random graph construction. This work investigates the phase transition properties of biomolecules and their implications in the evolutionary optimization in biopolymers. This role of random genotype-to-phenotype mappings in reducing the chance of being trapped in the suboptimal regions of the search space is explored in [67]. Experimental approaches to construct genetic regulatory networks are presented in [53].

The following section lays the foundation of the contribution of this paper. It presents a short review of orthonormal basis functions in the function space that will be useful in developing the proposed algorithms.

5 Distributed and Decomposed Representation of Functions

Describing a function first requires choosing a representation. Therefore, learning a function description also requires selecting a representation. In this paper we will consider representing functions using a weighted summation of certain kind of functions, called basis functions. Let Ξ be a set of basis functions. Let us index the basis functions in Ξ and denote the k-th basis function in Ξ by Ψ_k . Let I be the set of all such indices of the basis functions. A function $f(\mathbf{x})$ can be represented as,

$$f(\mathbf{x}) = \sum_{k \in I} w_k \Psi_k(\mathbf{x}) \tag{1}$$

Where $\Psi_k(\mathbf{x})$ denotes the k-th basis function and w_k denotes the corresponding coefficient. Although the structure of such functions may appear "simple", a properly chosen set of basis function should be able to represent any given function in the above form.

The objective of function induction can now be viewed as the task to generate a function, $\hat{f}(\mathbf{x}) = \sum_{k \in \hat{I}} \hat{w}_k \Psi_k(\mathbf{x})$, that approximates $f(\mathbf{x})$ from a given data set; \hat{I} denotes a subset of I; \hat{w}_k denotes the approximate estimation of the coefficients w_k . For a given basis representation, the underlying inductive task can be viewed as the problem to compute the non-zero, significant (not negligible) coefficients, \hat{w}_k -s. Let us illustrate this using a simple example. Consider a function of boolean variables, x_1, x_2 , and x_3 . We can write,

$$f(x_1, x_2, x_3) = w_0 + w_1 \Psi_1(x_1) + w_2 \Psi_2(x_2) + w_3 \Psi_3(x_3) + w_4 \Psi_4(x_1 x_2) +$$

$$w_5\Psi_5(x_1x_3) + w_6\Psi_6(x_2x_3) + w_7\Psi_7(x_1, x_2, x_3)$$

Where, w_i -s are constant coefficients; $\Psi_i(.)$ -s are monomial basis functions like Walsh functions [5, 76] to be defined later. At this point all we need to note is that we can write f as a linear sum of a set of basis functions, weighted by the corresponding basis coefficients. In other words, computation of $f(x_1, x_2, x_3)$ can be performed by computing different sub-functions that require only a subset of the feature set x_1, x_2, x_3 . Although computation of $\Psi_7(x_1, x_2, x_3)$ requires information about all the three variables, if the value of w_7 is close to zero then we can decompose the computation of $f(x_1, x_2, x_3)$ into different components that require only partial information about the feature set.

Distributed evaluation of fitness function is possible only when we have its representation using a set of basis functions and their corresponding coefficients. The distributed fitness evaluation in gene expression should be no exception. The efficacy of a certain portion of the DNA depends on the 3-dimensional structure of the protein it produces; since the shape of proteins depends on different physical factors such as energy, bond properties and others, the set of basis functions used in nature are likely to be functions of these physical factors. However, the exact mathematical structure of these basis functions is not yet known. The algorithms presented in the following part of this paper can be easily extended to any functionally complete basis set that satisfy some common closure properties that are satisfied by most of the common basis that we often deal with.

However, in the following discussion we choose to work with Walsh basis functions because of its existing connections to the field of genetic algorithms [8, 9, 14, 16, 17, 18, 26, 45, 58, 61]. Walsh basis is functionally complete over the space of all boolean strings. In other words it can represent any function that can be defined over the space of boolean strings. The following discussion offers a brief overview of Walsh representation.

Walsh functions [5, 76] are orthogonal functions that found applications in many different fields such as signal processing, image analysis, and others. Like Fourier, Laplace, and other transformations, Walsh functions are often used to represent a problem solving task in a convenient form. Application of Walsh transformation (WT) in understanding Genetic Algorithms was first noted by Bethke [7]. Further investigation of this approach can be found elsewhere [14, 16, 17, 26, 50, 61, 74, 75]. Traditionally, the Walsh functions are used for representing real valued functions of binary variables. However, they can be easily extended to higher cardinality representation, as shown elsewhere [58]. Although the main arguments of the following discussion can be extended for higher cardinality representations, in this paper we shall restrict ourselves to binary variables.

The Walsh basis set is comprised of 2^{ℓ} Walsh functions, where each basis function is defined as follows:

$$\psi_{\mathbf{j}}(\mathbf{x}) = (-1)^{(\mathbf{x}.\mathbf{j})}. \tag{2}$$

Where \mathbf{j} and \mathbf{x} are binary strings of length ℓ . In other words $\mathbf{j} = j_1, j_2, \dots j_\ell$, $\mathbf{x} = x_1, x_2, \dots x_\ell$ and $\mathbf{j}, \mathbf{x} \in \{0,1\}^\ell$. $\psi_{\mathbf{j}}(\mathbf{x})$ can either be 1 or -1. The string \mathbf{j} is called a partition. The order of partition \mathbf{j} is the number of 1-s in \mathbf{j} . A Walsh function depends on only those x_i -s only when $j_i = 1$. Therefore a partition can also be viewed as a representation of a certain subset of x_i -s; every unique partition corresponds to a unique subset of x_i -s. If a partition \mathbf{j} has exactly α number of 1-s then we say partition

is of order α since the corresponding Walsh function is a function of only those variables corresponding to the 1-s in the partition **j**. A function $f(\mathbf{x})$ can be written using the Walsh basis functions as follows:

$$f(\mathbf{x}) = \sum_{\mathbf{j}} w_{\mathbf{j}} \psi_{\mathbf{j}}(\mathbf{x}) \tag{3}$$

where $w_{\mathbf{j}}$ is the Walsh Coefficient (WC) corresponding to the partition \mathbf{j} . We can easily derive the following expression for WCs exploiting the orthonormality property of Walsh basis functions:

$$w_{\mathbf{j}} = \frac{1}{2^{\ell}} \sum_{\mathbf{x}} f(\mathbf{x}) \psi_{\mathbf{j}}(\mathbf{x})$$
 (4)

We note from Equation 3 that a function can be expressed as a linear sum of the Walsh functions, each weighed by the corresponding Walsh coefficients. The Walsh coefficient $w_{\mathbf{j}}$ can be viewed as the relative contribution of the partition \mathbf{j} to the function value of $f(\mathbf{x})$. Therefore, the absolute value of $w_{\mathbf{j}}$ can be used as the "significance" of the corresponding partition \mathbf{j} .

Partitions with non-zero Walsh coefficients capture the underlying structure of the given problem. For example, consider a function $f(x_1, x_2, x_3, x_4) = f_1(x_1, x_2) +$ $f_2(x_3, x_4)$. In the Walsh representation the values of w_{1111} , w_{1110} and any such other Walsh coefficient corresponding to partitions involving a pair of variables, one each from the two linearly decomposable partitions, are zero. Walsh functions can be used for representing any functions of boolean variables. If a function has dependencies among the features then its Walsh representation will reflect that and the function can be evaluated by computing the Walsh functions corresponding to the non-zero Walsh coefficients. If every variable in a function depends on every other variable then in the general case the Walsh representation will have all the 2^{ℓ} terms. On the other hand if at most some k variables interacts with each other, all the Walsh coefficients corresponding to partitions with more than k number of 1-s will be zero. This class of problems will be called problems with order-k level of interaction. Detection of such interaction among the genes is traditionally called *linkage learning* in the genetic algorithms literature. A perspective of linkage learning using Walsh representation has been proposed elsewhere [39, 71].

If the distributed fitness evaluation of the DNA through gene expression is a result of evolutionary search, then evolution must have a mechanism for constructing such a distributed representation of the fitness function. Walsh basis functions offer one way to decompose and distribute the fitness evaluation. Construction of such a representation in a relatively small period of time (in the evolutionary scale) is unlikely to happen unless it is fundamentally possible to do so in rigorous computational ground. The following section identifies a class of algorithms to efficiently construct such a representation.

6 Polynomial-Time Construction of Decomposed Representation

As we saw in the previous section (Equation 4) computation of a single Walsh Coefficient requires information about all the 2^{ℓ} domain members. Clearly this cannot be done in time, polynomial in ℓ . In order to make the problem tractable we are going to assume that the problem has bounded variable interaction of order-k. This is a reasonable assumption for many practical domains. This results in a sparse Walsh representation. In

general, function induction is fundamentally difficult if the orthonormal representation is not sparse [48]. Even if the problem has bounded order of interaction, explicit computation of WCs using Equation 4 requires exponential time. Another possibility is to generate $m = \sum_{z=0}^k \binom{\ell}{z}$ different members from the domain and solve a large $(m \times m)$ linear system of equations in order to compute the m possibly non-zero terms in the Walsh representation. Although it is theoretically possible in polynomial time, it is not clear how and if at all the evolutionary search is equipped with any mechanism to do it this way. In the following discussion we explore an alternate way to compute individual WCs in an efficient manner.

From Equation 3 we can write,

$$f(\mathbf{x})\psi_{\mathbf{i}}(\mathbf{x}) = \sum_{\mathbf{i}} w_{\mathbf{j}}\psi_{\mathbf{j}}(\mathbf{x})\psi_{\mathbf{i}}(\mathbf{x})$$

Let i be a partition and $S(\mathbf{i})$ be the set of all strings that satisfies the following conditions: (1) every member of $S(\mathbf{i})$ has same values at all positions where there is a 0 in i and (2) the substring defined by the positions corresponding to 1-s in i is unique in every member of $S(\mathbf{i})$. Let us denote the invariant values at the positions, corresponding to 0-s in i by T and call it the template ¹. For example, if $\mathbf{i} = 001100$ then one possible choice of S may be $\{000000,001000,00100,001100\}$. $|S(\mathbf{i})|$ is the size of the set $S(\mathbf{i})$ and $|S(\mathbf{i})| = 2^k$ when the partition i is of order-k. In this case the template $\mathbf{T} = 00$ __00. Since there exists different such $S(\mathbf{i})$ -s depending on the choice of \mathbf{T} , we choose to use the symbol $S_{\mathbf{T}}(\mathbf{i})$ to denote the set $S(\mathbf{i})$ with respect to certain template \mathbf{T} , wherever needed. Now we can write,

$$\sum_{\mathbf{x} \in S_{\mathbf{T}}(\mathbf{i})} f(\mathbf{x}) \psi_{\mathbf{i}}(\mathbf{x}) = \sum_{\mathbf{j}} w_{\mathbf{j}} \sum_{\mathbf{x} \in S_{\mathbf{T}}(\mathbf{i})} \psi_{\mathbf{j}}(\mathbf{x}) \psi_{\mathbf{i}}(\mathbf{x})$$

$$= \sum_{\mathbf{j} \in J(\mathbf{i})} w_{\mathbf{j}} \sum_{\mathbf{x} \in S_{\mathbf{T}}(\mathbf{i})} \psi_{\mathbf{j} \oplus \mathbf{i}}(\mathbf{x})$$

$$\sum_{\mathbf{j} \in J(\mathbf{i})} w_{\mathbf{j}} \sum_{\mathbf{x} \in S_{\mathbf{T}}(\mathbf{i})} \psi_{\mathbf{j} \oplus \mathbf{i}}(\mathbf{x}) = \sum_{\mathbf{x} \in S_{\mathbf{T}}(\mathbf{i})} f(\mathbf{x}) \psi_{\mathbf{i}}(\mathbf{x}) \tag{5}$$

Where $J(\mathbf{i})$ denotes the set of all partitions that completely subsumes partition i. In other words, every partition in $J(\mathbf{i})$ must have an 1 at every location where there is an 1 in \mathbf{i} . $\mathbf{j} \oplus \mathbf{i}$ denotes the partition defined by the boolean XOR between \mathbf{j} and \mathbf{i} .

The following section presents a simple, deterministic algorithm to compute the Walsh representation in polynomial time for problems with bounded non-linear dependencies among the search variables.

6.1 DR1: A Simple Deterministic Algorithm

Since we can choose any invariant set of values for the template, let us consider a special case where all the required values of the template are set to 0. Let us denote the $S_{\mathbf{T}}(\mathbf{i})$ corresponding to this special case template $\mathbf{T} = \mathbf{0}$ by $S_{\mathbf{0}}(\mathbf{i})$. Note that the example that we gave earlier follows this case. Equation 5 can be specialized for this case as follows.

$$\sum_{\mathbf{j} \in J(\mathbf{i})} w_{\mathbf{j}} = \frac{1}{|S_{\mathbf{0}}(\mathbf{i})|} \sum_{\mathbf{x} \in S_{\mathbf{0}}(\mathbf{i})} f(\mathbf{x}) \psi_{\mathbf{i}}(\mathbf{x})$$
(6)

¹The idea of using templates in the current context drew motivations from the messy GA literature [23].

Equation 6 can be used to efficiently detect the significant Walsh coefficients of the function with bounded non-linearity. Recall that for functions with at most k variables non-linearly interacting with each other, all the WCs corresponding to partitions with more than k number of 1-s will be zero. Therefore, for all partitions \mathbf{i} with more than k number of 1-s, the total number of non-zero coefficients in $J(\mathbf{i})$ is zero. For any partition with the order equal or more to k, we can write,

$$w_{\mathbf{i}} = \frac{1}{|S_{\mathbf{0}}(\mathbf{i})|} \sum_{\mathbf{x} \in S_{\mathbf{0}}(\mathbf{i})} f(\mathbf{x}) \psi_{\mathbf{i}}(\mathbf{x})$$
(7)

Note that the computation of w_i requires only 2^k evaluations of $f(\mathbf{x})$. The bounded non-linearity property can therefore be exploited to compute the WCs using only a small number of evaluations (2^k) compared to the usual 2^ℓ evaluations needed using the regular approach. Once we compute all the k-th order non-zero WCs using Equation 7, lower order coefficients can be computed using the known higher order coefficients and Equation 5. The main algorithmic steps of this technique can be summarized as,

- 1. select $k \leq \ell$, some constant that bounds the highest order non-linearity of the given problem;
- 2. compute the order-k WCs using Equation 7;
- 3. use Equation 5 and the already evaluated order-k WCs in order to compute order-(k-1) WCs; continue this process iteratively for $(k-1), (k-2), \cdots$ 1-order WCs; note that no additional function evaluation is needed after the order-k WCs are computed.

This technique can find all the non-zero WCs of a problem with order-k non-linearity in polynomial time using $2^k \binom{\ell}{k}$ function evaluations. The computation of individual WCs simply requires computing the average of 2^k fitness values and a few addition and subtraction. Although the complexity of this algorithm is polynomial in ℓ for problems with constant k, it is fairly expensive for many practical problems. The following section presents a very efficient, non-deterministic algorithm.

6.2 DR2: An Efficient, Non-Deterministic Algorithm

This section presents an algorithm to construct the distributed orthonormal representation by evaluating Equation 5 for a set of randomly generated templates. A random choice of template generates a particular assignment of signs of the corresponding Walsh term in Equation 5. For the special case $\mathbf{T} = \mathbf{0}$, every $\psi_{\mathbf{j} \oplus \mathbf{i}}(\mathbf{x}) = 1$. If all the coefficients corresponding to partitions that subsume a given partition \mathbf{i} are zero then the left hand side of Equation 5 must produce a zero for any choice of templates. If it returns a non-zero value then at least one of the coefficients in $S_{\mathbf{T}}(\mathbf{i})$ is non-zero. The proposed algorithm makes use of this observation.

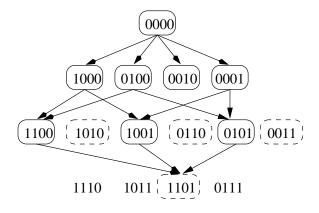
The algorithms searches for significant coefficients in the lattice of all partitions. The main steps are as follows:

- 1. Consider the lattice of all partitions, partially ordered based on the order of the partitions.
- 2. Start from the partition with zero order, i.e. the one with no fixed bit.

- 3. Traverse the lattice using a chosen order (e.g. depth-first or breadth-first). Initialize $\alpha = 0$. At each node do the following m number of times:
 - (a) Randomly generate a template.
 - (b) Compute $\sum_{\mathbf{x} \in S_{\mathbf{T}}(\mathbf{i})} f(\mathbf{x}) \psi_{\mathbf{i}}(\mathbf{x})$ at each node; if it returns a non-zero significant number then exit loop.
 - (c) Otherwise, set $\alpha = \alpha + 1$.
- 4. If $\alpha < m$ continue traversing new nodes using the chosen search strategy.
- 5. If $\alpha == m$ discard all the nodes subsumed by the current node from the scope of future search for nodes with significant coefficients.

The parameter m is user given. When m is large enough such that every possible template is considered for the test, Equation 5 is guaranteed to detect any non-zero coefficient corresponding to partitions that subsume the partition i. The reason behind this is the following. Note that for an ℓ -bit problem and an order-k partition i, there are $2^{\ell-k}$ possible choices of templates. On the other hand there are $2^{\ell-k}$ different partitions that subsume the partition i and therefore there are that many WCs. Clearly, we have $2^{\ell-k}$ unknown Walsh coefficients and $2^{\ell-k}$ different templates can generate that many equations. If all the tests or all the different templates return zero then we have a set of $2^{\ell-k}$ homogeneous equations. In that case the unknown WCs must take only the trivial solution i.e. all of them are zeros. Although the deterministically correct solution can be obtained only when we enumerate all the templates, a small value of m appears to suffice for many practical cases because of the following reason. Let ν be the proportion of templates at a given node for which $\sum_{\mathbf{x} \in S_{\mathbf{T}}(\mathbf{i})} f(\mathbf{x}) \psi_{\mathbf{i}}(\mathbf{x}) = 0$ despite the existence of non-zero contributing coefficients in the summation. Therefore the probability that all of the m experiments will return zero and thereby discard the node is ν^m . If $\nu < 1$ then the probability of such mistakes goes down exponentially with m. So a small value of m should be sufficient for all practical purposes. In fact, randomized sampling of a few templates was sufficient for all the experimental results presented later in this paper. The next section illustrates this algorithm using an example.

Consider the lattice of all sixteen partitions for a four-bit problem as shown in Figure 4. We are interested in a function for which only the partitions, encircled with solid lines, have non-zero WCs. The proposed algorithm first performs the significance test at all nodes for order-1 partitions. For this case, the test is expected to produce non-zero value at each of these nodes, indicating that the partition is subsumed by some partitions with non-zero WC. Next the algorithm considers the nodes at the third level from top in Figure 4. Since all the order-2 partitions subsume some set of order-1 partitions and all the order-1 partitions returned non-zero value for our test, we need to apply our test at every node corresponding to the order-2 partitions. Our test is expected to return non-zero values only for 1100, 1001, and 0101. Next we consider every unique order-3 partition that subsumes at least one of the partitions 1100, 1001, and 0101 but do not subsume any of the partitions 1010, 0110, and 0011. There is only one such partition and that is 1101. We again apply our test at this node and expect to observe that the test returns a zero value. Next we backtrack to the order-2 partition level and note that the outcomes of the tests that we performed earlier at each of these nodes are essentially the WC of the corresponding node since the coefficient of the partition 1101 is zero. Similarly, we continue to backtrack and compute the coefficients of every nonzero partition. This technique requires $O(2^k r)$ objective function evaluations, where



1111

Figure 4: Efficient detection of Walsh Coefficients.

r is the total number of non-zero WCs in its Walsh representation. The algorithm needs to evaluate all the nodes corresponding to the order-2 partitions. Therefore, the complexity of the should be at least quadratic in ℓ . For problems where r is $O(\ell^2)$ and k is a constant, the total number of objective function evaluations is $O(\ell^2)$.

Induction of a function in distributed representation is important in many domains like machine learning, optimization, data mining and many others. The algorithms proposed in this section can be applied to each of these application domains. The following section considers its application in optimization.

7 Application of DR2 in Linkage Learning

Evolutionary algorithms are widely used for optimization applications. Scalable optimization in absence of adequate knowledge about the search space requires efficient detection of the regularity and the underlying structure of the search space. The proposed algorithm can be efficiently used for this purpose. Detection of such structure has been traditionally called *linkage learning* [39] in the genetic algorithms literature.

Linkage learning algorithms try to detect the structure of the search space using similarity-based equivalence relations or partitions. If a set of search-variables together contribute significantly to the objective function, then the quality of the solution will also largely depend on the values set to the these variables. Therefore detection of such mutually interacting cluster of variables (i.e. the linkage among the variables) is important in optimization. Genetic algorithms-based optimization is no exception. Since the space of all such subset of variables or partitions is typically exponential in problem size (ℓ) , efficient detection of such significant variable interaction is very important for the scalability of the genetic algorithm.

For hard problems simple GA may not provide scalable performance because of this. It has been shown elsewhere [72, 70] that the time needed for the convergence to the optimal solution grows exponentially with the problem-size in absence of the knowledge regarding the important partitions. The genetic algorithm community have realized the

importance of linkage learning in the scalability of the genetic algorithm. A growing number of linkage-learning techniques [3, 4, 12, 23, 20, 24, 32, 31, 41, 54, 55, 56, 70] are becoming available. The following part of this section presents a brief review of some of the earlier efforts in linkage learning.

The history of linkage learning efforts dates back to Bagley's dissertation [2]. Bagley used a flexible representation and the so called *inversion* operator for adaptively clustering the related genes. Bagley did not conclude in favor of the use of inversion for linkage learning. Rosenberg [64] also investigated the possibility of learning linkage by evolving the probability of choosing a location for crossover. Frantz [15] also investigated the utility of the inversion operator and confirmed that inversion is too slow and not very effective. Schaffer and Morishima [66] introduced a set of flags in the representation. These flags were used for identifying the set of genes to be used for crossover points. They noted the formation of certain favorite crossover points in the population, that corroborated their hypothesis regarding the need for detecting gene linkage. Goldberg and Bridges [19] confirmed that lack of linkage knowledge can lead to failure of GAs for difficult classes of problems, such as deceptive problems. Additional efforts on linkage learning GAs can be found elsewhere [49, 59].

The messy GAs (mGAs) [12, 23, 21] tries to detect linkage by explicitly evaluating schemata [27] using a template (a solution string that is used for filling up the missing values corresponding to the wild card characters of a schema) and selecting good schemata through a selection-only primordial stage. This is a heuristic-based approach and often, its application is computationally expensive. The fast messy GA [22] offered some reduction in computational cost of linkage learning. As noted earlier, the idea of templates in the algorithms proposed in the current paper draws motivation from the templates in messy GAs.

Several new techniques have come up in the recent past. The gene expression messy GA (GEMGA) introduced elsewhere [4, 32, 31, 38] offered a technique for linkage learning. The GEMGA makes use of a local perturbation technique to identify the genes that are critical for high fitness. Once the genes are identified in the local context, they are put together in clusters and tested for global performance. Good clusters define the genetic linkage. This class of algorithms is also based on the local-perturbation heuristics. However the authors reported scalable $O(\ell^2)$ performance.

Harik introduced the Linkage Learning GA (LLGA) [25, 24]. The LLGA tries to learn linkage by exploiting the exchange crossover operator and the probabilistic expression based representation. The LLGA appears to work nicely particularly for problems in which construction of a linear ordering among the partitions is not so difficult. In a recent work [51] relations between compressed introns and the LLGA representation is discussed. Smith and Fogarty [68] reported a technique for evolving genetic linkage and to exploit it for adapting the recombination strategy. They reported superior performance of their linkage learning evolutionary algorithm over traditional GA.

A linkage learning approach similar to the GEMGA can be found elsewhere [44]. This approach makes use of a GEMGA-like filtering approach to detect the good partitions and schemata. In a recent work [57] a new linkage learning algorithm LINC is proposed. The LINC algorithm works by checking second order non-linearity. It considers feature pairs and performs $O(\ell^2)$ experiments. Let us define $\delta f_i = f(...\overline{x}_i...) - f(...x_i...)$, $\delta f_j = f(....\overline{x}_j...) - f(...x_j...)$, and $\delta f_{ij} = f(....\overline{x}_i\overline{x}_j...) - f(...x_ix_j...)$; where x_i is a boolean variable and $\overline{x}_i = 1 - x_i$. The LINC algorithm detects linkage by exploiting the fact

that if two features i and j have pair-wise non-linearity then $|\delta f_{ij} - \delta f_i - \delta f_j| > \epsilon$, where ϵ is a constant.

A principal component analysis based construction of representation for performing evolutionary optimization has been developed elsewhere [73]. Kazadi [43] proposed a similar approach to explicitly detect generalized schemata, that he calls conjugate schemata. His approach proposed a second order non-linearity detection technique in the continuous space, similar to what the recently proposed LINC algorithm uses in the discrete boolean space. A different technique for detecting the significant relations using a dependency tree-based approach has been proposed elsewhere [3]. This approach also exploits the second order non-linearity and estimates a second order approximation of the underlying relations; they reported superior performance of their algorithm over other techniques that do not explicitly try to search and exploit relations.

The approach proposed elsewhere [54, 55] is based on estimation of the underlying distribution function. However, since distribution estimation is a hard problem faced in many domains, their approach assumes prior knowledge about the structure of the distribution and reduces the task to estimation of the distribution parameters with known structure. However, their recent effort [] in this area addressed the issue of learning the search-space structure.

The possibility of linkage learning using Walsh coefficients was first noted elsewhere [35, 39]. Recently [70] also investigated the possibility of using the KM algorithms [48] for estimating the Walsh coefficients. However, the author reported scaling problem of the KM approach since it requires large number of function evaluations for correctly estimating the coefficients. The DR2 algorithm proposed in this paper share similarities with the KM-approach. Both of them explore the space of all partitions in a kind of divide-and-conquer approach; both of them are randomized algorithms. However, DR2 imposes a different lattice structure in the space of all partitions that draws motivations from the traditional notion of schema and templates. Unlike the KM-based approach, DR2-based linkage learning simply tries to detect existence of any non-zero coefficient down the path rooted at the current node.

The randomized algorithm DR2 can be directly used for constructing the Walsh representation in $O(2^k r)$ time. Once the representation is constructed we can easily identify the linkage among the genes by noting the relative magnitude of the coefficients. If a partition has a large magnitude the corresponding variables are strongly linked and they contribute to the objective function in a significant manner. On the other hand if a partition has a zero or relatively negligible coefficient then it does not contribute significantly to the objective function. Therefore, we can first run the proposed algorithm to detect the linkage and then make use of the linkage information to guide the genetic search in a fashion similar to earlier techniques [4, 32, 31, 33, 34, 35, 38]. In this paper we focus only on the former part since that is the primary challenge in front of the linkage-learning genetic algorithms. We have applied the proposed algorithm for detecting the linkage for several test functions. The following section reports the experimental results.

8 Experimental Results

The experimental results presented here report only the cost of detecting the underlying structure since it has already been shown elsewhere [4, 32, 31, 33, 34, 35, 38] that we can solve such problems using recombination and selection-like operators easily once the structure is correctly detected. These papers reported that the scalability of these

techniques critically depends on the complexity of the linkage learning algorithm. The results presented in the following sections demonstrate that the proposed randomized algorithm can be successfully used for linkage learning in any genetic algorithms for solving many optimization problems with bounded dependency in $O(\ell^2)$ time.

The experimental test-bed is comprised of problems with bounded dependency. All the objective functions are decomposable to a set of overlapping and non-overlapping sub-functions. For all test problems at most 5 variables can interact with each other. For all functions with overlapping sub-functions, any given sub-function shares one variable with one other sub-function. No prior knowledge about such decomposability is provided to the linkage-learning algorithm. The proposed algorithm DR2 is used for generating the decomposable representation. The experiments made use of two different ways to pick up the template. In the first case the template for computing the test at every node of the lattice was selected from prior preliminary experiments. In the second case a randomly generated template was used. The objectives behind presenting the results for these two different cases are: (1) to demonstrate that reducing a constant number of tests at every node does not change the underlying complexity and (2) if available, prior knowledge about the template can be incorporated into the algorithm for reducing the cost by a constant factor. A template of all 1-s and all 0-s are chosen for the former case. For the latter case, 10 randomly selected templates are used, which turned out to be sufficient for all test functions. DR2 could detect linkages without any mistake for all test functions using either one of these templates.

TRAP: A Deceptive Function

The deceptive trap [1] function is defined as, $f(\mathbf{x}) = k$ if u = k; $f(\mathbf{x}) = k - 1$ u otherwise; where u is the unitation variable, or the number of 1-s in the string x, and k is the length of the sub-function. If we carefully observe this trap function, we shall note that it has two peaks. One of them corresponds to the string with all 1-s (the global optima) and the other is the string with all 0-s (the suboptimal solution). The objective function is constructed by concatenating several deceptive trap functions one after another. The overall objective function is simply a weighted linear summation of the individual subfunctions. For uniformly scaled problems all the weights are set to 1. For non-uniformly scaled problems, weights vary through $1, 2, \dots \mu$, with the weight for the leftmost subfunction set to 1 and rightmost one set to μ . For $\ell = 200$, and k = 5, the overall function contains 40 sub-functions; therefore, an order-5 bounded 200-bit problem has 2^{40} local optima, and among them, only one is globally optimal. As the problem length increases the number of local optima exponentially increases. Figure 5 (Top) shows the growth of number of objective function evaluations with respect to increasing number of search variables. Pre-selected templates are used for these experiments.

MUH: The Muehlenbein Function

This function is defined in Table 1. The global optima is the string of all 0-s while all the strings having a number of trailing 1-s constitute the local optima. Unlike the case for *Trap*, here the building block corresponding to the global optima, has a significant amount of overlap with the local optima. Figure 5 (Bottom) shows the growth of number of objective function evaluations with respect to increasing number of search variables. Pre-selected templates are used for these experiments.

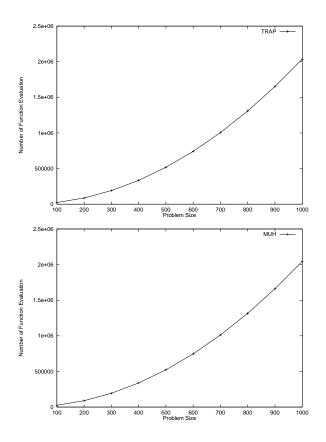


Figure 5: The number of function evaluation vs. problem size in detecting linkage in case of (Top) uniformly scaled non-overlapping TRAP and (Bottom) overlapping MUH using selected template. At most five variables can be mutually dependent.

Mühlenbein	GW2
f(x) = 4 if $x = 00000$	f(x) = 10 if u = 0
= 3 if $x = 00001$	= 8 if $u=k$
= 2 if $x = 00011$	= 7 if $u=1$ and $odd(0)$
= 1 if $x = 00111$	= 2 if $u=1$ and $even(1)$
= 0 if $x = 01111$	= 4 if $u=k-1$ and $odd(1)$
= 3.5 if x = 111111	= 3 if $u=k-1$ and $even(1)$
= 0 otherwise.	=0 otherwise.

Table 1: Functions odd(0) and even(0) return true if the number of 0-s in x are odd and even respectively. odd(1) and even(1) are analogously defined.

Multi-modal	GW1		
$f(x) = u + 2 \times f'(x)$	f(x) = 4	if	x = 1 # 1 # 0
where,		if	x = 1 # 0 # 0
f'(x) = 1 if odd(u)	= 10	if	x = 0 # 1 # 0
= 0 otherwise	= 0	if	x = 0 # 1 # 0

Table 2: (left) Massively multi-modal function and (right) GW1; u denotes the number of 1-s in the string. The symbol # denotes the don't care position.

GW1: Goldberg-Wang Function 1

This function is defined in Table 2. Figure 6 (Top) shows the growth of number of objective function evaluations with respect to increasing number of search variables.

GW2: Goldberg-Wang Function 2

This function is defined in Table 1. Figure 6 (Bottom) shows the growth of number of objective function evaluations with respect to increasing number of search variables.

MULTI: A Massively Multi-Modal Function

This is a massively multi-modal function of unitation where the global optima is a string of all 1's (assuming that length of the sub-function is odd). It is defined in Table 2. This function resembles a one-max function with "bumps". Figure 7 shows the growth of number of objective function evaluations with respect to increasing number of search variables.

The experimental results presented here clearly demonstrates the scalable $O(\ell^2)$ performance of the proposed randomized algorithm. Since the proposed approach is based on a well-grounded theoretical foundation, it should be equally applicable to other discrete objective functions. The following section discusses the future work and its connections to the biology.

9 Future Research Directions

The proposed stochastic algorithm for decomposed representation construction scales up when the number of mutually dependent genes is not greater than some small constant. Although this may be true for many fitness functions, it is easy to construct functions that do not satisfy this condition. Therefore, it is quite natural to ask the validity of

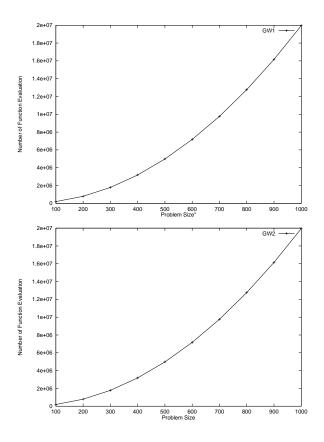


Figure 6: The number of function evaluation vs. problem size in detecting linkage in case of GW1 (Top) and GW2 (Bottom) with 10 randomized templates. Each graph represents results of both uniformly and linearly scaled non-overlapping cases. No difference in the number of function evaluation is noted between the uniformly and linearly scaled cases. At most five variables can be mutually dependent. For linearly scaled problem, the subfunctions are multiplied by $1, 2, 3 \cdots \mu$ with 1 being assigned to the leftmost subfunction and μ to the rightmost one..

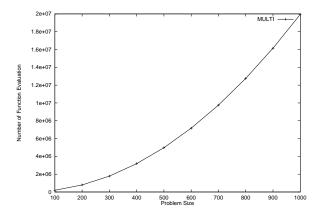


Figure 7: The number of function evaluation vs. problem size in detecting linkage in case of both uniformly scaled non-overlapping and overlapping MULTI with 10 randomized templates. No major difference in the number of function evaluation is noted between the non-overlapping and overlapping cases. At most five variables can be mutually dependent.

this assumption particularly in the context of gene expression. We need to justify this and we have reasons to believe that the justification may come from the way the gene expression process works. As noted earlier, this process involves several representation transformations. The translation (transformation of mRNA to Protein) is one among them. This transformation is controlled by the genetic code. Our recent work [36, 37] extended our approach by exploring the effect of genetic code-like representation transformations in the domain of binary strings. This paper shows that genetic codelike transformations introduce an interesting property in the representation of a genetic fitness function. It points out that such adaptive transformations can convert some functions with an exponentially large description in Walsh basis to one that is highly suitable for polynomial-size approximation. Such transformations can construct a Walsh representation with only a polynomial number of low-order terms that are exponentially more significant than the rest when fitter chromosomes are given more copies through a redundant, equivalent representation. This is a very desirable property [48, 29] for efficient function-induction from data which is a fundamental problem in learning, data mining, and optimization. This also means that in such representations higher order interactions among the variables are negligible. We still need to identify the class of functions for which such transformations will work. We also need to develop techniques for constructing such transformations in an evolutionary algorithm.

One alternate approach to the randomized technique proposed here is to transform the representation of the given objective function in such a way that all the Walsh coefficients are non-negative. In that case the summation of any subset of such coefficients will be equal to zero only when the coefficients are individually zero. From Equation 4 we can write,

$$w_{\mathbf{j}} = \sum_{\mathbf{x} \in \Omega^{+}(\mathbf{j})} f(\mathbf{x}) \psi_{\mathbf{j}}(\mathbf{x}) + \sum_{\mathbf{x} \in \Omega^{-}(\mathbf{j})} f(\mathbf{x}) \psi_{\mathbf{j}}(\mathbf{x})$$
(8)

where $\Omega^+(\mathbf{j})$ and $\Omega^-(\mathbf{j})$ define the set of all strings for which $\psi_{\mathbf{j}}(\mathbf{x})$ is 1 and -1 respectively. Clearly there exists a decomposition of any function $f(\mathbf{x}) = f_1(\mathbf{x}) - f_2(\mathbf{x})$ in such a way that both f_1 and f_2 have non-negative WCs. Note that this requires controlled generation of \mathbf{x} -s such that the corresponding basis functions for a given j return either all positive or all negative. This simple construction shows that it is always possible to transform a given function so that all the WCs are non-negative. A simple way to do that is to translate the $f(\mathbf{0})$ value by some large enough positive constant, ρ . Since $\psi_{\mathbf{j}}(\mathbf{0}) = 1$ such translation will translate every WC by the amount $\frac{\rho}{2^d}$. If ρ is large enough then all the WCs will be non-negative. Although this makes our algorithm applicable, the problem is that this may destroy the underlying sparseness of the coefficients. In other words, coefficients that were originally zero will become non-zero because of the translation. This may give rise to an exponential value of r and as a result the algorithm may no longer remain computable in polynomial time.

An alternate approach to address this problem is to manipulate the representation in such a way that the coefficients become non-negative without destroying the sparseness. It is not clear how to do that. However, it is interesting to observe that complementary alphabet transformations (like what we see in transcription) offer some control over the basis functions that may be useful.

Let \mathbf{x} be a binary string and let \mathcal{T} be a complementary operator that maps 1 to 0 and vice versa. Let $\mathcal{T}_{\beta}(\mathbf{x})$ be the complementary transformation applied on the β -partition of \mathbf{x} . In other words, $\mathcal{T}_{\beta}(\mathbf{x})$ complements only those positions of \mathbf{x} where there is a 1 in β . Let us now consider the difference between the Walsh function $\psi_{\beta}(\mathcal{T}_{\beta}(\mathbf{x}))$ and $\psi_{\beta}(\mathbf{x})$. Recall that $\psi_{\beta}(\mathbf{x})$ can be either -1 or 1. It turns out that $\psi_{\beta}(\mathcal{T}_{\beta}(\mathbf{x})) = \psi_{\beta}(\mathbf{x})$ when the number of transcribed features is even; on the other hand $\psi_{\beta}(\mathcal{T}_{\beta}(\mathbf{x})) = -\psi_{\beta}(\mathbf{x})$ when the number of 1-s in β ; g_1 and g_0 be the numbers of 1-s and 0-s in \overline{x} within the partition defined by the 1-s in β . The number of ones in $\mathcal{T}_{\beta}(\mathbf{x})$ within the partition β , $g'_1 = g_0 = g - g_1$. Now if both g and g_1 are even numbers then g'_1 must be even. On the other hand if g and g_1 are even and odd numbers respectively then g'_1 must be odd. In other words the sign of $\psi_{\beta}(\overline{x})$ does not change when \overline{x} is transformed to a different string by applying \mathcal{T} over an even number of bits. Consider $\psi_{0110}(101) = -1$. Now if we apply \mathcal{T} to the underscored bits we get $\psi_{0110}(1101) = -1$. A similar rationale can be developed for the case when g is odd.

Now consider a transformation of the representation of the domain in such a way that every \mathbf{x} is represented by $\mathcal{T}_1(\mathbf{x})$, where $\mathbf{1}$ is an ℓ -bit string of 1-s. Such representation flips the sign of the WC corresponding to every odd-order partition. However, it does not destroy the sparseness; WCs with a value of zero, remain zero. We may be able to exploit such complementation-based representation transformation techniques for computing the summation of all non-negative coefficients. However, this is only our hypothesis since this is similar to the physical representation transformations in transcription at an abstract level.

The current implementation of the proposed algorithm works in a centralized fashion. In other words it generates the distributed, decomposed representation by searching in a centrally constructed lattice of partitions. Work on extending this algorithm to a hierarchical, distributed computing-based approach is also on progress. In this approach the partitions defined by different subsets of features are explored in parallel. This work is likely to make the proposed approach suitable for distributed computing environments.

10 Conclusions

This paper notes that fitness evaluation in natural evolution takes place in a distributed fashion in different living cells through the process of gene expression. It argues that such distributed evaluation of the fitness is only possible when the function can be correctly decomposed into different sub-functions. Unless such a representation was available a priori, we have every reason to believe that there must be an efficient mechanism to compute such a distributed, decomposed representation. It develops techniques to do that in polynomial time. It proposes an efficient randomized algorithm to construct such representation of a function when the number of mutually interacting variables is bounded by a constant. Although we could have presented the algorithms without any reference to the gene expression process, we choose not to do so because of our continuing effort to understand this process from the perspective of evolutionary search. We think a presentation from a pure algorithm design perspective without any reference to biology will unnecessarily restrict the scope of our research.

It is important to note that the requirement of bounded order of interaction has deep implication in polynomial complexity search [48]; without that common machine learning and optimization will be quite useless in the general case, as long as polynomialtime computation is desired. For example, consider a decision tree [60]. Even such a popular inductive learning algorithm may engage in an exponential-time tree-construction in absence of this requirement, in the worst case producing a tree that is no better than table-look-up. Bounded order of dependence among the search variables guarantees a tree of bounded depth and thereby a polynomial-time computability. This assumption is reasonable and most importantly practical. However, as noted earlier genetic code-like transformations may further extend the scope of the proposed algorithms by constructing a representation of some functions where the higher order coefficients are negligible. For problems that satisfy this condition, the proposed algorithm guarantees linear-time performance with respect to r with a probabilistic notion of correctness. Although this paper did not directly relate the proposed randomized approach to a specific mechanisms of gene expression, this work and the previous papers along this line have established that polynomial-time computation of the distributed representation of the objective function is possible under reasonable assumption. Now that we have a strong foundation, the next step is to investigate the implications of the specific transformations in gene expression.

Acknowledgments

This work was supported by the United States National Science Foundation Grant IIS-9803660.

References

- D. H. Ackley. A connectionist machine for genetic hill climbing. Kluwer Academic, Boston, 1987.
- [2] J. D. Bagley. The behavior of adaptive systems which employ genetic and correlation algorithms. *Dissertation Abstracts International*, 28(12):5106B, 1967. (University Microfilms No. 68-7556).
- [3] S. Baluja and S. Davies. Using optimal dependency-trees for combinatorial optimization: Learning the structure of the search space. Technical Report CMU-CS-

- 97-107, Department of Computer Science, Carnegie Mellon University, Pittsburgh, 1997.
- [4] S. Bandyopadhyay, H. Kargupta, and G. Wang. Revisiting the GEMGA: Scalable evolutionary optimization through linkage learning. In *Proceedings of the IEEE In*ternational Conference on Evolutionary Computation, pages 603–608. IEEE Press, 1998.
- [5] K. G. Beauchamp. Applications of Walsh and Related Functions. Academic Press, USA, 1984.
- [6] R. Belew and M. Vose, editors. Foundations of Genetic Algorithms, San Mateo, CA, 1996. Morgan Kaufmann.
- [7] A. D. Bethke. Comparison of genetic algorithms and gradient-based optimizers on parallel processors: Efficiency of use of processing capacity. Tech. Rep. No. 197, University of Michigan, Logic of Computers Group, Ann Arbor, 1976.
- [8] A. D. Bethke. Genetic algorithms as function optimizers. *Dissertation Abstracts International*, 41(9):3503B, 1981. (University Microfilms No. 8106101).
- [9] C. L. Bridges and D. E. Goldberg. The nonuniform Walsh-schema transform. In G. J. E. Rawlins, editor, Foundations of Genetic Algorithms, pages 13–22. 1991.
- [10] A. Brindle. Genetic Algorithms for Function Optimization. Unpublished doctoral dissertation, University of Alberta, Edmonton, Canada, 1981.
- [11] D. Dasgupta and D. R. McGregor. Designing neural networks using the structured genetic algorithm. *Artificial Neural Networks*, 2:263–268, 1992.
- [12] K. Deb. Binary and floating-point function optimization using messy genetic algorithms. IlliGAL Report no. 91004 and doctoral dissertation, University of Alabama, Tuscaloosa, University of Illinois at Urbana-Champaign, Illinois Genetic Algorithms Laboratory, Urbana, 1991.
- [13] L. J. Fogel, A. J. Owens, and M. J. Walsh. Artificial Intelligence through Simulated Evolution. John Wiley, New York, 1966.
- [14] S. Forrest and M. Mitchell. The performance of genetic algorithms on Walsh polynomials: Some anomalous results and their explanation. In R. K. Belew and L. B. Booker, editors, *Proceedings of the Fourth International Conference on Genetic Algorithms*, pages 182–189. Morgan Kaufmann, San Mateo, CA, 1991.
- [15] D. R. Frantz. Non-linearities in genetic adaptive search. *Dissertation Abstracts International*, 33(11):5240B-5241B, 1972. (University Microfilms No. 73-11,116).
- [16] D. E. Goldberg. Genetic algorithms and Walsh functions: Part I, a gentle introduction. *Complex Systems*, 3(2):129–152, 1989. (Also TCGA Report 88006).
- [17] D. E. Goldberg. Genetic algorithms and Walsh functions: Part II, deception and its analysis. *Complex Systems*, 3(2):153–171, 1989. (Also TCGA Report 89001).

- [18] D. E. Goldberg. Construction of high-order deceptive functions from low-order Walsh coefficients. IlliGAL Report No. 90002, University of Illinois at Urbana-Champaign, Illinois Genetic Algorithms Laboratory, Urbana, 1990.
- [19] D. E. Goldberg and C. L. Bridges. An analysis of a reordering operator on a GA-hard problem. *Biological Cybernetics*, 62:397–405, 1990. (Also TCGA Report No. 88005).
- [20] D. E. Goldberg, K. Deb, H. Kargupta, and G. Harik. Rapid, accurate optimization of difficult problems using fast messy genetic algorithms. *Proceedings of the Fifth International Conference on Genetic Algorithms*, pages 56-64, 1993.
- [21] D. E. Goldberg, K. Deb, and B. Korb. Messy genetic algorithms revisited: Studies in mixed size and scale. *Complex Systems*, 4:415–444, 1990.
- [22] D. E. Goldberg, K. Deb, and B. Korb. Don't worry, be messy. In R. K. Belew and L. B. Booker, editors, Proceedings of the Fourth International Conference on Genetic Algorithms, pages 24–30. Morgan Kaufmann, San Mateo, CA, 1991.
- [23] D. E. Goldberg, B. Korb, and K. Deb. Messy genetic algorithms: Motivation, analysis, and first results. *Complex Systems*, 3(5):493–530, 1989. (Also TCGA Report 89003).
- [24] G. Harik. Learning Linkage to Efficiently Solve Problems of Bounded Difficulty Using Genetic Algorithms. PhD thesis, Department of Computer Science, University of Michigan, Ann Arbor, 1997.
- [25] G. Harik and D. E. Goldberg. Learning linkage. In Belew and Vose [6].
- [26] R. Heckendorn and D. Whitley. Predicting epistasis from mathematical models. Journal Of Evolutionary Computation, 7(1):69–101, 1999.
- [27] J. H. Holland. Adaptation in Natural and Artificial Systems. University of Michigan Press, Ann Arbor, 1975.
- [28] R. B. Hollstien. Artificial genetic adaptation in computer control systems. *Dissertation Abstracts International*, 32(3):1510B, 1971. (University Microfilms No. 71-23,773).
- [29] J. Jackson. The Harmonic Sieve: A Novel Application of Fourier Analysis to Machine Learning Theory and Practice. PhD thesis, School of Computer Science, Carnegie Mellon University, Pittsburgh, PA, 1995.
- [30] F. Jacob and J. Monod. Genetic regulatory mechanisms in the synthesis of proteins. Molecular Biology, 3:318–356, 1961.
- [31] H. Kargupta. SEARCH, Computational Processes in Evolution, and Preliminary Development of the Gene Expression Messy Genetic Algorithm. *Complex Systems*, 11(4):233–287, 1997.
- [32] H. Kargupta. The gene expression messy genetic algorithm. In *Proceedings of the IEEE International Conference on Evolutionary Computation*, pages 814–819. IEEE Press, 1996.

- [33] H. Kargupta. Gene expression: The missing link of evolutionary computation. In C. Poloni D. Quagliarella, J. Periaux and G. Winter, editors, *Genetic Algorithms in Engineering and Computer Science.*, page Chapter 4. John Wiley & Sons Ltd., 1997.
- [34] H. Kargupta, D. E. Goldberg, and L. W. Wang. Extending the class of order-k delineable problems for the gene expression messy genetic algorithm. In *Proceedings* of the Second Annual Conference on Genetic Programming, pages 364–369. Morgan Kaufmann Publishers, 1997.
- [35] H. Kargupta. Gene expression and large scale evolutionary optimization. In Computational Aerosciences in the 21st Century. Kluwer Academic Publishers, 1998.
- [36] H. Kargupta. A striking property of genetic code-like transformations. School of EECS Technical Report EECS-99-004, Washington State University, Pullman, WA, 1999. http://www.eecs.wsu.edu/~hillol/gene_expression.html.
- [37] H. Kargupta. Genetic code-like transformations and their effect on learning functions. In *Parallel Problem Solving from Nature*, pages 99–108. Springer, 2000. Extended version is in communication.
- [38] H. Kargupta and S. Bandyopadhyay. Further experimentations on the scalability of the GEMGA. In *Lecture Notes in Computer Science: Parallel Problem Solving from Nature*, pages 315–324. Springer-Verlag, 1998.
- [39] H. Kargupta and S. Bandyopadhyay. A perspective on the foundation and evolution of the linkage learning genetic algorithms. *Computer Methods in Applied Mechanics and Engineering*, 186(2000):269–294, 2000. Special Issue on Genetic Algorithms, Guest Editors: Goldberg, D. E. and Deb, K.
- [40] H. Kargupta and D. E. Goldberg. SEARCH, blackbox optimization, and sample complexity. In Belew and Vose [6], pages 291–324.
- [41] H. Kargupta and K. Sarkar. Function induction, gene expression, and evolutionary representation construction. In *Proceedings of the Genetic and Evolutionary Computation Conference*, Orlando, USA. AAAI Press., pages 313–320. Morgan Kaufmann, 1999.
- [42] S. Kauffman. The Origins of Order. Oxford University Press, New York, 1993.
- [43] S. Kazadi. Conjugate schema in genetic search. In *Proceedings of the International Conference on Genetic Algorithms*, pages 10–25, 1997. Morgan Kaufmann.
- [44] C. Kemenade. Explicit filtering of building blocks and genetic algorithms. Personal communication, August 1996.
- [45] S. Khuri. Walsh and Haar functions in genetic algorithms. Proceedings of the 1994 ACM Symposium on Applied Computing, pages 201-205, 1994.
- [46] S. Kirpatrick, C. D. Gelatt, and M. P. Vecchi. Optimization by simulated annealing. Science, 220(4598):671–680, 1983.

- [47] J. R. Koza. Genetic programming: On programming computers by means of natural selection and genetics. MIT Press, Cambridge, MA, 1992.
- [48] S. Kushilevitz and Y. Mansour. Learning decision trees using Fourier spectrum. In *Proc. 23rd Annual ACM Symp. on Theory of Computing*, pages 455–464, 1991.
- [49] J. R. Levenick. Inserting introns improves genetic algorithm success rate: Taking a cue from biology. In R. K. Belew and L. B. Booker, editors, *Proceedings of the Fourth International Conference on Genetic Algorithms*, pages 123–127. Morgan Kaufmann, San Mateo, CA, 1991.
- [50] G. E. Liepins and M. D. Vose. Polynomials, basic sets, and deceptiveness in genetic algorithms. *Complex Systems*, 5(1):45–61, 1991.
- [51] F. Lobo, K. Deb, D. Goldberg, G. Harik, and L. Wang. Compressed introns in a linkage learning genetic algorithms. In *Genetic Programming: Proceedings of* the Third Annual Conference, pages 551–558, San Francisco, CA, 1998. Morgan Kaufmann.
- [52] R. S. Michalski. Theory and methodology of inductive learning. In R. S. Michalski, J. G. Carbonell, and T. M. Mitchell, editors, *Machine learning: An artificial intelligence approach*, pages 323–348. Tioga Publishing Co, 1983.
- [53] M. Morohashi and H. Kitano. Identifying gene regulatory networks from time series expression data by *in silico* sampling and screening. In *Proceedings of the 5th European Conference on Artificial Life*, pages 477–486. Springer, 1999.
- [54] H. Mühlenbein and G. Paab. From recombination of genes to the estimation of distributions I. binary parameters. In *Parallel Problem Solving from Nature - PPSN IV*, pages 178–187, Berlin, 1996. Springer.
- [55] H. Mühlenbein and A. O. Rodriguez. Schemata, distributions and graphical models in evolutionary optimization. Personal Communication., December 1997.
- [56] H. Mühlenbein and T. Mahnig. FDA a scalable evolutionary algorithm for the optimization of additively decomposed functions. *Journal of Evolutionary Computation*, 7(4):353–376, 1999.
- [57] M. Munetomo and D. E. Goldberg. Linkage Identification by Non-monotonicity Detection for Overlapping Functions Journal of Evolutionary Computation, 7(4):377–398, 1999.
- [58] C. K. Oei. Walsh function analysis of genetic algorithms of nonbinary strings. Unpublished master's thesis, Urbana, 1992. University of Illinois at Urbana-Champaign, Department of Computer Science.
- [59] J. Paredis. The symbolic evolution of solutions and their representations. In L. Eshelman, editor, *Proceedings of the Sixth International Conference on Genetic Algorithms*, pages 359–365, San Mateo, CA, 1995. Morgan Kaufmann.
- [60] J. R. Quinlan. Induction of decision trees. Machine Learning, 1(1):81–106, 1986.

- [61] S. Rana, R. B. Heckendorn, and D. Whitley. A tractable Walsh analysis of SAT and its implications for genetic algorithms. In *Proceedings of the AAAI-98*, 1998. AAAI Press.
- [62] I. Rechenberg. Kybernetische lösungsansteuerung einer experimentellen forschungsaufgabe. Seminarvortrag, Hermann-Föttinger-Institut für Strömungstechnik der Technische Universität, Berlin, 1964.
- [63] C. Reidys and S. Fraser. Evolution of random structures. Technical Report 96-11-082, Santa Fe Institute, Santa Fe, 1996.
- [64] R. S. Rosenberg. Simulation of genetic populations with biochemical properties. *Dissertation Abstracts International*, 28(7):2732B, 1967. (University Microfilms No. 67-17,836).
- [65] D. E. Rumelhart, J. L. McClelland, and the PDP Research Group. Parallel Distributed Processing: Explorations in the Microstructure of Cognition, Vol 1: Foundations. MIT Press, Cambridge, Mass., 1 edition, 1986.
- [66] J. D. Schaffer and A. Morishima. An adaptive crossover distribution mechanism for genetic algorithms. In J. J. Grefenstette, editor, *Proceedings of the Second International Conference on Genetic Algorithms*, pages 36–40. 1987.
- [67] M. Shackleton, R. Shipman, and M. Ebner. An investigation of redundant genotype-phenotype mappings and their role in evolutionary search. In *Proceedings* of the 2000 Congress on Evolutionary Computation, pages 493–500, Los Alamitos, California, USA, 2000. IEEE Press.
- [68] J. Smith and T. Fogarty. Recombination strategy adaptation via evolution of gene linkage. In Proceedings of the IEEE International Conference on Evolutionary Computation, pages 826–831. IEEE Press, 1996.
- [69] R. E. Smith. An investigation of diploid genetic algorithms for adaptive search of non-stationary functions. TCGA Report No. 88001, University of Alabama, The Clearinghouse for Genetic Algorithms, Tuscaloosa, 1988.
- [70] D. Thierens. Estimating the significant non-linearities in the genome problem-coding. In *Proceedings of the Genetic and Evolutionary Computation Conference*, pages 643–648. Morgan Kaufmann Publishers, 1999.
- [71] D. Thierens. Scalability problems of simple genetic algorithms. *Evolutionary Computation*, 7(4):331–352, 1999.
- [72] D. Thierens and D. Goldberg. Mixing in genetic algorithms. In S. Forrest, editor, Proceedings of the Fifth International Conference on Genetic Algorithms, pages 38–45, San Mateo, CA, 1993. Morgan Kaufmann.
- [73] H. Voigt and H. Muhlenbein. Gene pool recombination and the utilization of covariances for the breeder genetic algorithm. In *Proceedings of the Second International Conference on Evolutionary Computation*, pages 172–177, 1995. New York: IEEE Press.

- [74] M. Vose and A. Wright. The simple genetic algorithm and the Walsh transform: Part I, theory. *Journal of Evolutionary Computation*, 6(3):253–274, 1998.
- [75] M. Vose and A. Wright. The simple genetic algorithm and the Walsh transform: Part II, the inverse. *Journal of Evolutionary Computation*, 6(3):253–274, 1998.
- [76] J. L. Walsh. A closed set of orthogonal functions. Ann. Journ. Math., 55, 1923.