

Generalized Walsh Transforms and Epistasis

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Abstract

In this note, we introduce and briefly study a non-binary analogue of the “classical” Walsh transform. It is shown that this transform allows to rewrite the definition of normalized epistasis in terms of generalized Walsh coefficients, in a way which is both practical and elegant. Some examples are included, aiming to give a first indication of the strength of this approach.

Introduction

The classical genetic algorithm (GA) starts from a fitness function f , i.e., a positive real-valued function f on $\Omega = \{0, 1\}^\ell$ (the set of all length ℓ strings $s = s_{\ell-1} \dots s_0$), and aims to find its maximum (or minimum). There are many factors which may make a fitness function hard to optimize by a genetic algorithm, one of them being the existence of relations or links between separate bits, cf. [2], for example. In [7] Rawlins compares this phenomenon to a similar situation in genetics, where a gene at some locus in the chromosome may hide the (phenotypical) effect of another gene at a different locus, cf. [8]. When this phenomenon occurs, one refers to the first gene as being *epistatic* to the second one.

Adapting this idea to the framework of GAs, Rawlins speaks of *minimal epistasis* when every bit in a string is independent of any other one, i.e., when the fitness function f may basically be given as a linear combination of functions, each of which only depends upon a single bit. At the other extreme, we have *maximal epistasis*, if no proper subset of genes is independent of any other gene, and this situation corresponds to f essentially being a random function.

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The quantification of these ideas considered in [9, 10, 11] extends ideas of Davidor [1], and consists in associating to any fitness function f on $\{0, 1\}^\ell$ a positive value $\varepsilon(f)$ in such a way that $\varepsilon(f) = 0$ corresponds to minimal epistasis. In [5], these ideas are generalized to more general, not necessarily binary alphabets and fitness functions with minimal resp. maximal epistasis are explicitly described.

In the first section of the present note, we recall how previous definitions of epistasis [1, 7] may be reshaped into a more precise, algebraic form and we introduce, in particular, the notion of “normalized epistasis” $\varepsilon^*(f)$ of a fitness function f acting on strings over a not necessary binary alphabet. In the second section, we define generalized (complex) Walsh transforms and show how these, and their “classical” counterpart, allow for an easier calculation of normalized epistasis. We illustrate this, in the third section, by applying our methods to particular instances of fitness functions, like ordinary and generalized unitation functions as well as some other elementary examples.

1 Epistasis

1.1 Throughout this text, we work over a fixed alphabet A of cardinality n , which we usually identify with the set of integers $\{0, \dots, n-1\}$. The set A^ℓ consisting of all length ℓ strings $s = s_{\ell-1} \cdots s_0$ over A will be denoted by Ω . Let \mathbb{R}_+ denote the set of all positive real numbers. *Fitness functions* are maps $f : \Omega \rightarrow \mathbb{R}_+$, (which we want to optimize!). Mimicking ideas due to Davidor [1] in the binary case, the epistasis $\varepsilon(s)$ of a string s in a population $P \subseteq \Omega$ may be defined as follows.

Denote by

$$f_P = \frac{1}{|P|} \sum_{s \in P} f(s)$$

the average fitness of f over P and for any $0 \leq i < \ell$ and $a \in A$ by

$$f_{P(a,i)} = \frac{1}{|P(a,i)|} \sum_{s \in P(a,i)} f(s)$$

the average fitness over $P(a,i)$, the sub-population consisting of all strings $s_{\ell-1} \cdots s_0 \in P$ with $s_i = a$. The epistasis of a string s over a population P is defined as

$$\varepsilon_P(s) = f(s) - \sum_{i=0}^{\ell-1} \frac{1}{|P(s_i, i)|} \sum_{t \in P(s_i, i)} f(t) + \frac{\ell-1}{|P|} \sum_{t \in P} f(t).$$

In this note, we will only be working with the full search space Ω , so $|P| = n^\ell$ and the previous formula simplifies to

$$\varepsilon(s) = f(s) - \sum_{i=0}^{\ell-1} \frac{1}{n^{\ell-1}} \sum_{t \in \Omega(s_i, i)} f(t) + \frac{\ell-1}{n^\ell} \sum_{t \in \Omega} f(t),$$

where $\Omega(a, i)$ now consists, for any $a \in A$, of all strings in Ω having value a at the i th position. In this case, the *global epistasis* of f is defined to be

$$\varepsilon_{n,\ell}(f) = \sqrt{\sum_{s \in \Omega} \varepsilon^2(s)}.$$

1.2 As in [5, 9], the previous definition may be rewritten in a more elegant form. Indeed, consider the vectors

$$\mathbf{e} = \begin{pmatrix} \varepsilon(0 \dots 00) \\ \varepsilon(0 \dots 01) \\ \vdots \\ \varepsilon((n-1)^{(\ell)}) \end{pmatrix} \text{ resp. } \mathbf{f} = \begin{pmatrix} f_0 \\ \vdots \\ f_{n^\ell-1} \end{pmatrix},$$

where $(n-1)^{(\ell)}$ is the length ℓ string all of whose components have value $(n-1)$, and where we write $f_0, \dots, f_{n^\ell-1}$ for $f(0 \dots 00), \dots, f((n-1)^{(\ell)})$.

For any positive integers $0 \leq i, j \leq n^\ell - 1$, let us put

$$e_{ij} = \frac{1}{n^\ell} ((n-1)\ell + 1 - nd_{ij}),$$

where d_{ij} (or d_{ij}^n , if ambiguity may arise) is the (n -ary) Hamming distance between i and j , i.e., the number of “bits” in which the n -ary representations of i and j differ. For example, $d_{16,24}^3 = 2$, since, in ternary notation, $16 = 121$ and $24 = 220$. Putting $\mathbf{E}_{n,\ell} = (e_{ij}) \in M_{n^\ell}(\mathbb{Q})$, the square matrices of dimension n^ℓ with rational entries, it is easy to see that

$$\mathbf{e} = \mathbf{f} - \mathbf{E}_{n,\ell} \mathbf{f}.$$

This allows us to define the *global epistasis* of f to be

$$\varepsilon_{n,\ell}(f) = \|\mathbf{e}\| = \|\mathbf{f} - \mathbf{E}_{n,\ell} \mathbf{f}\|.$$

Usually, one prefers to work with the integer matrix $\mathbf{G}_{n,\ell} = n^\ell \mathbf{E}_{n,\ell}$ with entries $g_{ij} = (n-1)\ell + 1 - nd_{ij}$ for all $0 \leq i, j \leq n^\ell - 1$. This matrix may also be defined inductively by

$$\mathbf{G}_\ell = \begin{pmatrix} \mathbf{G}_{\ell-1} + (n-1)\mathbf{U}_{\ell-1} & \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} \\ \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} & \mathbf{G}_{\ell-1} + (n-1)\mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} \\ \vdots & \vdots & \ddots & \vdots \\ \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} & \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{n,\ell-1} + (n-1)\mathbf{U}_{\ell-1} \end{pmatrix},$$

where we wrote \mathbf{G}_ℓ for $\mathbf{G}_{n,\ell}$ and where, for any positive integer k , the n^k -dimensional matrix $\mathbf{U}_k = \mathbf{U}_{n,k}$ is given by

$$\mathbf{U}_{n,k} = \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix}.$$

A straightforward induction argument, using the previous recursive formula, shows that $\mathbf{G}_{n,\ell}^2 = n^\ell \mathbf{G}_{n,\ell}$, hence that $\mathbf{E}_{n,\ell}$ is idempotent. Using this and the fact that $\mathbf{E}_{n,\ell}$ is symmetric, it follows that $\varepsilon_{n,\ell}^2(f) = {}^t \mathbf{f} (\mathbf{I}_{n,\ell} - \mathbf{E}_{n,\ell}) \mathbf{f}$, where $\mathbf{I}_{n,\ell}$ is the n^ℓ -dimensional identity matrix.

1.3 It is obvious that for any positive real number $r \in \mathbb{R}$, we have $\varepsilon_{n,\ell}(rf) = r\varepsilon_{n,\ell}(f)$, whereas the epistasis of f and rf , viewed as expressing linkage between different “bits”, should be the same. This leads one to define the *normalized epistasis* of a fitness function f as

$$\varepsilon_{n,\ell}^*(f) = \varepsilon_{n,\ell}^2 \left(\frac{f}{\|\mathbf{f}\|} \right) = \frac{\varepsilon_{n,\ell}^2(f)}{\|\mathbf{f}\|^2} = \frac{t\mathbf{f}(\mathbf{I}_{n,\ell} - \mathbf{E}_{n,\ell})\mathbf{f}}{t\mathbf{f}\mathbf{f}},$$

and, as $\mathbf{E}_{n,\ell}$ is an orthogonal projection, it thus follows that

$$0 \leq \varepsilon_{n,\ell}^*(f) \leq 1.$$

Actually, one may show that $\varepsilon_{n,\ell}^*(f) = 0$ is equivalent to f having minimal epistasis, in the sense of Rawlins [7]. On the other hand, it has been proved in [5] that the maximal value of $\varepsilon_{n,\ell}^*(f)$ that may be reached by a positive valued fitness function f is $1 - \frac{1}{n^{\ell-1}}$. In fact, this value is reached precisely by the fitness functions which are zero everywhere, except for n points at maximal Hamming distance and with equal fitness value. In particular, in the binary case ($n = 2$) the maximal value for the normalized epistasis, $1 - \frac{1}{2^{\ell-1}}$, is reached by so-called “camel functions”, i.e., fitness functions f with the property that there exists some $t \in \{0, 1\}^\ell$ with binary complement \hat{t} and some positive real number α such that $f(t) = f(\hat{t}) = \alpha$ and $f(s) = 0$ for $s \neq t, \hat{t}$.

2 The Generalized Walsh Transform

2.1 In this section, we define the generalized (complex) Walsh transform and we show how it may be used as a tool which allows for an easier calculation of the epistasis of a fitness function. Although our ideas are inspired by those of Goldberg [3], who successfully applied Walsh analysis to calculate schema averages, we will use a slightly different terminology.

Let r be a primitive root of unity. i.e., $r = e^{\frac{2\pi}{n}i} = \cos(\frac{2\pi}{n}) + i \sin(\frac{2\pi}{n})$. We define the set of complex vectors $\{\mathbf{v}_0, \mathbf{v}_1, \dots, \mathbf{v}_{n-1}\}$ by

$$\mathbf{v}_k = {}^t(1, r^k, r^{2k}, \dots, r^{(n-1)k}) \in \mathbb{C}^n$$

for all $0 \leq k \leq n - 1$.

Let us denote by $\mathbf{V}_{n,1}$ the (symmetric!) n -dimensional complex matrix given by

$$\mathbf{V}_{n,1} = (\mathbf{v}_0\mathbf{v}_1 \cdots \mathbf{v}_{n-1}).$$

For small values of n , we have $\mathbf{V}_{1,1} = (1)$ and

$$\mathbf{V}_{2,1} = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \in M_2(\mathbb{C}) \text{ resp. } \mathbf{V}_{3,1} = \begin{pmatrix} 1 & 1 & 1 \\ 1 & r & r^2 \\ 1 & r^2 & r \end{pmatrix} \in M_3(\mathbb{C})$$

where $r = -\frac{1}{2} + i\frac{\sqrt{3}}{2}$.

Let us take a moment to recall that the Kronecker product (or tensor product) $\mathbf{A} \otimes \mathbf{B}$ of any pair of matrices $\mathbf{A} = (a_{ij}) \in \mathbb{R}^{m \times n}$ and $\mathbf{B} = (b_{kl}) \in \mathbb{R}^{p \times q}$, is the matrix $(a_{ij}\mathbf{B})_{ij} \in \mathbb{R}^{mp \times nq}$, i.e.,

$$\mathbf{A} \otimes \mathbf{B} = \begin{pmatrix} a_{11}\mathbf{B} & \cdots & a_{1n}\mathbf{B} \\ \vdots & \ddots & \vdots \\ a_{m1}\mathbf{B} & \cdots & a_{mn}\mathbf{B} \end{pmatrix}.$$

In particular, we may thus put $\mathbf{A}^{\otimes m} = \mathbf{A} \otimes \cdots \otimes \mathbf{A}$ (m copies). Note that, obviously, ${}^t(\mathbf{A} \otimes \mathbf{B}) = {}^t\mathbf{A} \otimes {}^t\mathbf{B}$ and $(\mathbf{A} \otimes \mathbf{B})(\mathbf{C} \otimes \mathbf{D}) = (\mathbf{A}\mathbf{C}) \otimes (\mathbf{B}\mathbf{D})$, for all $\mathbf{A}, \mathbf{C} \in \mathbb{R}^{m \times m}$ and $\mathbf{B}, \mathbf{D} \in \mathbb{R}^{p \times p}$. For any complex matrices $\mathbf{A} \in \mathbb{C}^{m \times m}$ and $\mathbf{B} \in \mathbb{C}^{p \times p}$ we also have that $\overline{\mathbf{A} \otimes \mathbf{B}} = \overline{\mathbf{A}} \otimes \overline{\mathbf{B}}$.

With these definitions, let us put $\mathbf{V}_{n,\ell} = \mathbf{V}_{n,1}^{\otimes \ell}$, for any positive integer ℓ .

Lemma. 2.2 *For any positive integer ℓ , we have*

$$\overline{\mathbf{V}}_{n,\ell} \mathbf{V}_{n,\ell} = n^\ell \mathbf{I}_{n,\ell}$$

where $\overline{\mathbf{V}}_{n,\ell}$ denotes the adjoint complex matrix of $\mathbf{V}_{n,\ell}$.

Proof. The assertion is true for $\ell = 1$ because

$$(\overline{\mathbf{V}}_{n,1} \mathbf{V}_{n,1})_{ij} = \sum_{k=0}^{n-1} r^{n-ik} r^{jk} = \sum_{k=0}^{n-1} r^{k(j-i)} = \begin{cases} n & \text{if } i = j \\ 0 & \text{if } i \neq j. \end{cases}$$

The general case follows from a straightforward induction argument on ℓ , using the previous result:

$$\begin{aligned} \overline{\mathbf{V}}_{n,\ell} \mathbf{V}_{n,\ell} &= \overline{\mathbf{V}_{n,1}^{\otimes \ell} \mathbf{V}_{n,1}^{\otimes \ell}} = \overline{(\mathbf{V}_{n,1}^{\otimes (\ell-1)} \otimes \mathbf{V}_{n,1})} (\mathbf{V}_{n,1}^{\otimes (\ell-1)} \otimes \mathbf{V}_{n,1}) \\ &= (\overline{\mathbf{V}_{n,\ell-1}} \otimes \overline{\mathbf{V}_{n,1}}) (\mathbf{V}_{n,\ell-1} \otimes \mathbf{V}_{n,1}) \\ &= (\overline{\mathbf{V}_{n,\ell-1}} \mathbf{V}_{n,\ell-1}) \otimes (\overline{\mathbf{V}_{n,1}} \mathbf{V}_{n,1}) \\ &= n^{\ell-1} \mathbf{I}_{n,\ell-1} \otimes n \mathbf{I}_{n,1} = n^\ell \mathbf{I}_{n,\ell}. \end{aligned}$$

■

In order to prepare for the calculation of normalized epistasis in terms of generalized Walsh coefficients, let us first prove:

Lemma. 2.3 *For any positive integer ℓ , we have*

$$\overline{\mathbf{V}}_{n,\ell} \mathbf{U}_{n,\ell} \mathbf{V}_{n,\ell} = n^{2\ell} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}.$$

Proof. Let us again argue by induction on ℓ . The statement holds true for $\ell = 1$, because

$$\begin{aligned} \overline{\mathbf{V}}_{n,1} \mathbf{U}_{n,1} \mathbf{V}_{n,1} &= \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & r^{n-1} & \cdots & r \\ \vdots & \vdots & \ddots & \vdots \\ 1 & r & \cdots & r^{n-1} \end{pmatrix} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ 1 & r & \cdots & r^{n-1} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & r^{n-1} & \cdots & r^{(n-1)^2} \end{pmatrix} \\ &= \begin{pmatrix} n^2 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}. \end{aligned}$$

Now, assume the assertion is true up to $\ell - 1$ and let us prove it for ℓ . Then,

$$\begin{aligned} \overline{\mathbf{V}}_{n,\ell} \mathbf{U}_{n,\ell} \mathbf{V}_{n,\ell} &= \overline{(\mathbf{V}_{n,1}^{\otimes \ell})} \mathbf{U}_{n,\ell} (\mathbf{V}_{n,1}^{\otimes \ell}) \\ &= \overline{(\mathbf{V}_{n,1}^{\otimes (\ell-1)} \otimes \mathbf{V}_{n,1})} (\mathbf{U}_{n,\ell-1} \otimes \mathbf{U}_{n,1}) (\mathbf{V}_{n,1}^{\otimes (\ell-1)} \otimes \mathbf{V}_{n,1}) \\ &= (\overline{\mathbf{V}}_{n,\ell-1} \mathbf{U}_{n,\ell-1} \mathbf{V}_{n,\ell-1}) \otimes (\overline{\mathbf{V}}_{n,1} \mathbf{U}_{n,1} \mathbf{V}_{n,1}) \\ &= n^{2(\ell-1)} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \otimes n^2 \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \\ &= n^{2\ell} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}. \end{aligned}$$

■

We may now prove:

Lemma. 2.4 *With notations as before, we have:*

$$\overline{\mathbf{V}}_{n,\ell} \mathbf{G}_{n,\ell} \mathbf{V}_{n,\ell} = \mathbf{D}_{n,\ell},$$

where $\mathbf{D}_{n,\ell}$ is the diagonal matrix whose only non-zero diagonal entries d_{ii} have value $n^{2\ell}$ and are situated at $i = kn^j$, for values $0 \leq k < n$ and $0 \leq j < \ell$.

Proof. Using the recursive description of $\mathbf{G}_{n,\ell}$ given before, one easily deduces that

$$\mathbf{G}_{n,\ell} = \mathbf{U}_{n,1} \otimes \mathbf{G}_{n,\ell-1} + (\mathbf{G}_{n,1} - \mathbf{U}_{n,1}) \otimes \mathbf{U}_{n,\ell-1}.$$

It thus follows that

$$\overline{\mathbf{V}}_{n,\ell} \mathbf{G}_{n,\ell} \mathbf{V}_{n,\ell} = \mathbf{A} + \mathbf{B}$$

where

$$\mathbf{A} = \overline{\mathbf{V}}_{n,\ell} (\mathbf{U}_{n,1} \otimes \mathbf{G}_{n,\ell-1}) \mathbf{V}_{n,\ell}$$

resp.

$$\mathbf{B} = \overline{\mathbf{V}}_{n,\ell} ((\mathbf{G}_{n,1} - \mathbf{U}_{n,1}) \otimes \mathbf{U}_{n,\ell-1}) \mathbf{V}_{n,\ell}.$$

Let us now calculate these matrices \mathbf{A} and \mathbf{B} . First, using the fact that

$$\mathbf{V}_{n,\ell} = \mathbf{V}_{n,1} \otimes \mathbf{V}_{n,\ell-1},$$

let us note that

$$\begin{aligned} \mathbf{A} &= (\overline{\mathbf{V}}_{n,1} \otimes \overline{\mathbf{V}}_{n,\ell-1}) (\mathbf{U}_{n,1} \otimes \mathbf{G}_{n,\ell-1}) (\mathbf{V}_{n,1} \otimes \mathbf{V}_{n,\ell-1}) \\ &= (\overline{\mathbf{V}}_{n,1} \mathbf{U}_{n,1} \mathbf{V}_{n,1}) \otimes (\overline{\mathbf{V}}_{n,\ell-1} \mathbf{G}_{n,\ell-1} \mathbf{V}_{n,\ell-1}) \\ &= n^2 \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \otimes (\overline{\mathbf{V}}_{n,\ell-1} \mathbf{G}_{n,\ell-1} \mathbf{V}_{n,\ell-1}) \\ &= n^2 \begin{pmatrix} \overline{\mathbf{V}}_{n,\ell-1} \mathbf{G}_{n,\ell-1} \mathbf{V}_{n,\ell-1} & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}. \end{aligned}$$

On the other hand,

$$\begin{aligned} \mathbf{B} &= (\overline{\mathbf{V}}_{n,1} \otimes \overline{\mathbf{V}}_{n,\ell-1}) ((\mathbf{G}_{n,1} - \mathbf{U}_{n,1}) \otimes \mathbf{U}_{n,\ell-1}) (\mathbf{V}_{n,1} \otimes \mathbf{V}_{n,\ell-1}) \\ &= (\overline{\mathbf{V}}_{n,1} (\mathbf{G}_{n,1} - \mathbf{U}_{n,1}) \mathbf{V}_{n,1}) \otimes (\overline{\mathbf{V}}_{n,\ell-1} \mathbf{U}_{n,\ell-1} \mathbf{V}_{n,\ell-1}) \\ &= (n \overline{\mathbf{V}}_{n,1} \mathbf{V}_{n,1} - \overline{\mathbf{V}}_{n,1} \mathbf{U}_{n,1} \mathbf{V}_{n,1}) \otimes (\overline{\mathbf{V}}_{n,\ell-1} \mathbf{U}_{n,\ell-1} \mathbf{V}_{n,\ell-1}) \\ &= \left[n^2 \mathbf{I}_{n,1} - \begin{pmatrix} n^2 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \right] \otimes n^{2(\ell-1)} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix} \\ &= n^{2\ell} \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 \end{pmatrix} \otimes \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 \end{pmatrix}. \end{aligned}$$

Using this, another straightforward induction argument finishes the proof. \blacksquare

2.5 By analogy with the binary case (see [3, 6] for example), we define the (generalized) Walsh transform w of f by $\mathbf{w} = \mathbf{W}_{n,\ell} \mathbf{f}$, with $\mathbf{W}_{n,\ell} = n^{\frac{\ell}{2}} \mathbf{V}_{n,\ell}$. The (complex!) components $w_i = w_i(f)$ of \mathbf{w} will be called *generalized Walsh coefficients* of f . These coefficients, of course, easily permit to recover f , since it follows from $\overline{\mathbf{W}}_{n,\ell} \mathbf{W}_{n,\ell} = \mathbf{I}_{n,\ell}$ that

$$\mathbf{f} = \overline{\mathbf{W}}_{n,\ell} (\mathbf{W}_{n,\ell} \mathbf{f}) = \overline{\mathbf{W}}_{n,\ell} \mathbf{w}.$$

We may now prove:

Proposition. 2.6 *If $w_0, \dots, w_{n^\ell-1}$ are the generalized Walsh coefficients of the fitness function f , then the normalized epistasis $\varepsilon_{n,\ell}^*(f)$ of f is given by*

$$\varepsilon_{n,\ell}^*(f) = 1 - \frac{|w_0|^2 + \sum_{i=0}^{\ell-1} \sum_{k=1}^{n-1} |w_{k \cdot n^i}|^2}{\sum_{i=0}^{n^\ell-1} |w_i|^2}.$$

Proof. Since $\mathbf{f} = \overline{\mathbf{W}}_{n,\ell} \mathbf{w} = \mathbf{W}_{n,\ell} \overline{\mathbf{w}}$, we obtain that

$${}^t \mathbf{f} \mathbf{f} = {}^t (\overline{\mathbf{W}}_{n,\ell} \mathbf{w}) \mathbf{W}_{n,\ell} \overline{\mathbf{w}} = {}^t \mathbf{w} \overline{\mathbf{W}}_{n,\ell} \mathbf{W}_{n,\ell} \overline{\mathbf{w}} = {}^t \mathbf{w} \overline{\mathbf{w}},$$

as $\mathbf{W}_{n,\ell}$ is symmetric and $\overline{\mathbf{W}}_{n,\ell} \mathbf{W}_{n,\ell} = \mathbf{I}_{n,\ell}$. On the other hand,

$${}^t \mathbf{f} \mathbf{E}_{n,\ell} \mathbf{f} = n^{-\ell} {}^t (\overline{\mathbf{W}}_{n,\ell} \mathbf{w}) \mathbf{G}_{n,\ell} \mathbf{W}_{n,\ell} \overline{\mathbf{w}} = n^{-2\ell} {}^t \mathbf{w} \mathbf{D}_{n,\ell} \overline{\mathbf{w}}.$$

It thus follows that

$$\varepsilon_{n,\ell}^*(f) = 1 - \frac{{}^t \mathbf{f} \mathbf{E}_{n,\ell} \mathbf{f}}{{}^t \mathbf{f} \mathbf{f}} = 1 - \frac{{}^t \mathbf{w} \mathbf{D}_{n,\ell} \overline{\mathbf{w}}}{n^{2\ell} {}^t \mathbf{w} \overline{\mathbf{w}}}$$

and this equals $1 - \frac{|w_0|^2 + \sum_{i=0}^{\ell-1} \sum_{k=1}^{n-1} |w_{kn^i}|^2}{\sum_{i=0}^{n^\ell-1} |w_i|^2}$, indeed. ■

2.7 Let us now briefly consider the particular case $n = 2$. In this case, $\Omega = \{0, 1\}^\ell$, the space of binary strings of length ℓ , and $r = -1$. It follows that $\mathbf{V}_{2,\ell}$ (or just \mathbf{V}_ℓ) is given by $\mathbf{V}_\ell = \mathbf{V}_1^{\otimes \ell}$, where

$$\mathbf{V}_1 = \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix} \in M_2(\mathbb{Z}).$$

So \mathbf{V}_ℓ may inductively be constructed by

$$\mathbf{V}_\ell = \begin{pmatrix} \mathbf{V}_{\ell-1} & \mathbf{V}_{\ell-1} \\ \mathbf{V}_{\ell-1} & -\mathbf{V}_{\ell-1} \end{pmatrix} \in M_{2^\ell}(\mathbb{Z}).$$

The Walsh function ψ_t over $\{0, 1\}^\ell$ have been considered in [6] and are defined as

$$\psi_t(s) = \prod_{i=0}^{\ell-1} (-1)^{s_i t_i}$$

for any $s = s_{\ell-1} \dots s_0 \in \Omega$. It follows that ψ_t essentially counts for any string s the number of ones situated at loci where t also has value one. If $s \cdot t$ denotes the bitwise product of s and t , it is clear that $\psi_t(s) = (-1)^{s \cdot t}$. So, the Walsh functions may be represented by the matrix

$$(\psi_t(s))_{s,t \in \Omega} = \mathbf{V}_\ell.$$

Moreover, in [6] the authors define the Walsh transform $w = w(f)$ of f by its associated vector $\mathbf{w} = \mathbf{W}_\ell \mathbf{f}$, where \mathbf{W}_ℓ is the idempotent matrix given by $\mathbf{W}_\ell = 2^{-\frac{\ell}{2}} \mathbf{V}_\ell$ (see [6] for further details). As the Walsh functions form a basis for the vector space of real valued functions on $\{0, 1\}^\ell$, the components $w_i = w_i(f)$ of \mathbf{w} , the *Walsh coefficients of f* , are (up to a factor $2^{-\ell/2}$) the coordinates of f with respect to the basis $\{\psi_t; t \in \Omega\}$. The Walsh coefficients of f easily permit to recover f ; in fact

$$\mathbf{f} = \mathbf{W}_\ell(\mathbf{W}_\ell \mathbf{f}) = \mathbf{W}_\ell \mathbf{w}.$$

Moreover, in [6] it has been proved that $\mathbf{W}_\ell \mathbf{E}_\ell \mathbf{W}_\ell = \widetilde{\mathbf{D}}_\ell$ where $\widetilde{\mathbf{D}}_\ell$ (or $2^{-2\ell} \mathbf{D}_{2,\ell}$ with our notation) is the diagonal matrix, whose only non-zero diagonal entries d_{ii} have value 1 and are situated at $i = 0$ and $i = 2^j$, for $0 \leq j \leq \ell - 1$.

The general result above thus yields:

Proposition. 2.8 *If $w_0, \dots, w_{2^\ell-1}$ are the Walsh coefficients of the fitness function f , then the normalized epistasis $\varepsilon_{2,\ell}^*(f)$ of f is given by*

$$\varepsilon_{2,\ell}^*(f) = 1 - \frac{w_0^2 + \sum_{i=0}^{\ell-1} w_{2^i}^2}{\sum_{j=0}^{2^\ell-1} w_j^2}.$$

3 Some Examples

In this section, we describe some examples which illustrate how the previous results may be applied in order to effectively calculate the epistasis of some given fitness function.

3.1 As we pointed out in Section 1, it has been proved in [9] (in the binary case) and in [5] (in the general case) that a fitness function f has $\varepsilon^*(f) = 0$ if and only if f has minimal epistasis in the sense of [7], i.e., if f may be written in the form

$$f(s) = \sum_{i=0}^{\ell-1} g_i(s)$$

for some fitness functions g_i over \mathbb{R} , which only depend on the i -th bit.

Let us show how our approach allows for an easy proof of this result.

From the expression of normalized epistasis in terms of generalized Walsh coefficients, it follows that $\varepsilon_{n,\ell}^*(f) = 0$ is equivalent to $w_j = 0$ for all $j \neq 0, kn^i$ ($1 \leq k < n$, $0 \leq i < \ell$).

Here, $w_0 = n^{-\frac{\ell}{2}} \sum_{s \in \Omega} f(s)$, the average fitness value of f , just as in the binary case. As for the other terms, first note that $\mathbf{V}_{n,\ell}$ can also be given as $(r^{s \cdot t})_{s,t \in \Omega}$, where we denote by $s \cdot t$ the bitwise product of s and t modulo n , in accordance with

the binary case. So,

$$\begin{aligned}
w_{kn^i} &= n^{-\frac{\ell}{2}} \sum_{t \in \Omega} r^{kn^i \cdot t} f(t) = n^{-\frac{\ell}{2}} \sum_{t \in \Omega} r^{k \cdot t_i} f(t) \\
&= n^{-\frac{\ell}{2}} \left(\sum_{t \in \Omega(i,0)} f(t) + \sum_{t \in \Omega(i,1)} r^k f(t) + \cdots + \sum_{t \in \Omega(i,n-1)} r^{k(n-1)} f(t) \right) \\
&= n^{\frac{\ell}{2}-1} \sum_{j=0}^{n-1} r^{kj} f_{(i,j)}
\end{aligned}$$

where $f_{(i,j)} = \frac{1}{n^{\ell-1}} \sum_{t \in \Omega(i,j)} f(t)$, for all $j \in \{0, 1, \dots, n-1\}$.

It thus follows that $\varepsilon_{n,\ell}^*(f) = 0$ is equivalent to

$$\begin{aligned}
f(s) &= \left(\overline{\mathbf{W}}_{n,\ell} \mathbf{w} \right)_s = n^{-\frac{\ell}{2}} \left(\overline{\mathbf{V}}_{n,\ell} \mathbf{w} \right)_s = n^{-\frac{\ell}{2}} \sum_{t \in \Omega} r^{-s \cdot t} w_t \\
&= n^{-\frac{\ell}{2}} w_0 + n^{-\frac{\ell}{2}} \sum_{i=0}^{\ell-1} \sum_{k=1}^{n-1} r^{-s \cdot kn^i} w_{kn^i} = n^{-\frac{\ell}{2}} \left(w_0 + \sum_{i=0}^{\ell-1} \sum_{k=1}^{n-1} r^{-ks_i} w_{kn^i} \right) \\
&= n^{-\frac{\ell}{2}} \sum_{i=0}^{\ell-1} \left(\frac{w_0}{\ell} + \sum_{k=1}^{n-1} r^{-ks_i} w_{kn^i} \right) = \sum_{i=0}^{\ell-1} h_i(s),
\end{aligned}$$

where $h_i(s) = n^{-\frac{\ell}{2}} \left(\frac{w_0}{\ell} + \sum_{k=1}^{n-1} r^{-ks_i} w_{kn^i} \right) \in \mathbb{C}$, for all i . Actually,

$$f(s) = \sum_{i=0}^{\ell-1} h_i(s) = \sum_{i=0}^{\ell-1} \overline{h_i(s)} \in \mathbb{R},$$

so, $f(s) = \sum_{i=0}^{\ell-1} g_i(s)$, with

$$\begin{aligned}
g_i(s) &= \frac{1}{2} \left(h_i(s) + \overline{h_i(s)} \right) = n^{-\frac{\ell}{2}} \left[\frac{w_0}{\ell} + \frac{1}{2} \sum_{k=1}^{n-1} \left(r^{-ks_i} w_{kn^i} + r^{ks_i} \overline{w_{kn^i}} \right) \right] \\
&= n^{-\frac{\ell}{2}} \frac{w_0}{\ell} + \frac{1}{2n} \sum_{k=1}^{n-1} \left(\sum_{j=0}^{n-1} \left(r^{k(j-s_i)} + r^{k(s_i-j)} \right) f_{(i,j)} \right) \\
&= n^{-\frac{\ell}{2}} \frac{w_0}{\ell} + \frac{1}{n} \sum_{k=1}^{n-1} \sum_{j=0}^{n-1} \left(\cos \frac{2k(j-s_i)\pi}{n} \right) f_{(i,j)},
\end{aligned}$$

which clearly belongs to \mathbb{R} .

3.2 As another example, let us start by considering the set of vectors $\{\mathbf{e}_0, \dots, \mathbf{e}_{n-1}\}$ in \mathbb{R}^{n^ℓ} , with $\mathbf{e}_k = {}^t(0 \cdots 010 \cdots 0)$ where 1 appears as $k \frac{n^\ell-1}{n-1}$ -th coordinate, for $0 \leq k < n$. If we inductively define the set of complex vectors $\{\mathbf{v}_{0,\ell}, \dots, \mathbf{v}_{n^\ell-1,\ell}\}$ in \mathbb{C}^{n^ℓ} by putting $\mathbf{v}_{k,0} = 1$ for all k and, inductively,

$$\mathbf{v}_{k,\ell} = {}^t \left({}^t \mathbf{v}_{k,\ell-1}, r^k {}^t \mathbf{v}_{k,\ell-1}, r^{2k} {}^t \mathbf{v}_{k,\ell-1}, \dots, r^{(n-1)k} {}^t \mathbf{v}_{k,\ell-1} \right),$$

then $\mathbf{V}_{n,\ell} \mathbf{e}_k = \mathbf{v}_{k \frac{n^\ell-1}{n-1}, \ell}$, for all $0 \leq k < n$.

Let us now consider “generalized camel” functions, i.e., fitness functions defined by $f(s) = 0$ for all $s \in \Omega$, different from a chosen set of strings c_0, c_1, \dots, c_{n-1} in Ω which are pairwise at Hamming distance ℓ , and with $f(c_0) = f(c_1) = \dots = f(c_{n-1}) = 1$. In order to calculate their normalized epistasis, we may assume $c_0 = 0$ and so, $c_k = k \frac{n^\ell - 1}{n-1}$, ($1 \leq k < n$). Then, the vector associated to f is $\sum_{k=0}^{n-1} \mathbf{e}_k$. The generalized Walsh coefficients of f are thus given by

$$\mathbf{w} = \mathbf{W}_{n,\ell} \mathbf{f} = \mathbf{W}_{n,\ell} \sum_{k=0}^{n-1} \mathbf{e}_k = n^{\frac{-\ell}{2}} \sum_{k=0}^{n-1} \mathbf{V}_{n,\ell} \mathbf{e}_k = n^{\frac{-\ell}{2}} \sum_{k=0}^{n-1} \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell}.$$

It follows that

$$\begin{aligned} {}^t \mathbf{w} \overline{\mathbf{w}} &= \left(n^{\frac{-\ell}{2}} \sum_{k=0}^{n-1} {}^t \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell} \right) \left(n^{\frac{-\ell}{2}} \sum_{j=0}^{n-1} \overline{\mathbf{v}_{j \frac{n^\ell - 1}{n-1}, \ell}} \right) \\ &= n^{-\ell} \left(\sum_{k=0}^{n-1} \left| \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell} \right|^2 + 2 \sum_{k < j} {}^t \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell} \overline{\mathbf{v}_{j \frac{n^\ell - 1}{n-1}, \ell}} \right). \end{aligned}$$

But, $|\mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell}|^2 = n^\ell$, for all $0 \leq k < n$. In fact, as $\mathbf{v}_{k \frac{n^\ell - 1}{n-1}, 0} = (1)$, a straightforward induction argument on ℓ , proves that:

$$\begin{aligned} \left| \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell} \right|^2 &= {}^t \overline{\mathbf{v}}_{k \frac{n^\ell - 1}{n-1}, \ell} \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell} = \sum_{i=0}^{n-1} \left(r^{-ik \frac{n^\ell - 1}{n-1}} {}^t \overline{\mathbf{v}}_{k \frac{n^\ell - 1}{n-1}, \ell-1} r^{i \cdot k \frac{n^\ell - 1}{n-1}} \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell-1} \right) \\ &= \sum_{i=0}^{n-1} {}^t \overline{\mathbf{v}}_{k \frac{n^\ell - 1}{n-1}, \ell-1} \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell-1} = n \left| \mathbf{v}_{k \frac{n^\ell - 1}{n-1}, \ell-1} \right|^2 = n \cdot n^{\ell-1} = n^\ell. \end{aligned}$$

On the other hand, a similar argument as above shows that

$${}^t \overline{\mathbf{v}}_{k \frac{n^\ell - 1}{n-1}, \ell} \mathbf{v}_{j \frac{n^\ell - 1}{n-1}, \ell} = {}^t \overline{\mathbf{v}}_{k \frac{n^\ell - 1}{n-1}, \ell-1} \mathbf{v}_{j \frac{n^\ell - 1}{n-1}, \ell-1} \sum_{i=0}^{n-1} r^{i(j-k) \frac{n^\ell - 1}{n-1}} = 0,$$

if $k \neq j$. It now easily follows that ${}^t \mathbf{w} \overline{\mathbf{w}} = n$.

Moreover, one may verify, for example through an induction argument, that $w_{kn^i} = 0$ for all $1 \leq k < n$ and $0 \leq i < \ell$ and, as $w_0 = n^{\frac{-\ell}{2}+1}$, we finally have that

$$\varepsilon_{n,\ell}^*(f) = 1 - \frac{1}{n^{\ell-1}}$$

in accordance with the remarks made in Section 1.

3.3 As a final example, we consider so-called *generalized unitation functions*. These are fitness functions f with the property that there exist some functions g_i on $\{0, \dots, \ell - 1\}$, ($i = 0, \dots, n - 1$), with the property that $f(s) = \sum_{i=0}^{n-1} g_i(u_i(s))$ where, for any $s \in \Omega$, we denote by $u_i(s)$ the number of i 's in the n -ary representation of s , i.e., $u_i(s) = \#\{j; s_j = i\}$. In the particular case $n = 2$, we can rewrite f as

$$\begin{aligned} f(s) &= g_0(u_0(s)) + g_1(u_1(s)) \\ &= g_0(\ell - u_1(s)) + g_1(u_1(s)) \\ &= g(u(s)) \end{aligned}$$

with $g(\alpha) = g_0(\ell - \alpha) + g_1(\alpha)$ and $u(s) = u_1(s)$ is the unitation of s , i.e., the number of ones in the binary representation of s — for further details we refer to [4].

Let us fix some unitation function f , and denote by $w_0, \dots, w_{n^{\ell-1}}$ the associated generalized Walsh coefficients. Since for any permutation $\sigma(s)$ of s we obviously have $f(s) = f(\sigma(s))$, it is clear that $f_{(i,j)}$ is independent of i , and as $w_{kn^i} = n^{\frac{\ell}{2}-1} \sum_{j=0}^{n-1} r^{kj} f_{(i,j)}$, with notations as in 3.1, for each $k \in \{0, \dots, n-1\}$, we have

$$w_k = w_{kn} = w_{kn^2} = \dots = w_{kn^{\ell-1}} = \beta_k.$$

In order to write a general expression of $f_{(i,j)}$, let us consider the case $n = 3$ and then deduce the formula for the general case. Let us start with

$$f_{(i,0)} = \frac{1}{3^{\ell-1}} \sum_{s \in \Omega(0,0)} f(s) = \frac{1}{3^{\ell-1}} \sum_{s \in \Omega(0,0)} (g_0(u_0) + g_1(u_1) + g_2(u_2))$$

with $u_i = u_i(s)$, for $i = 0, 1, 2$.

If we take any $0 \leq a \leq \ell$ and $0 \leq b \leq \ell - a$, then it is clear that there are $\binom{\ell-1}{a-1} \binom{\ell-a}{b}$ strings in $\Omega(0,0)$ with $u_0 = a$, $u_1 = b$ and $u_2 = \ell - a - b$. This yields that

$$\begin{aligned} f_{(i,0)} &= \frac{1}{3^{\ell-1}} \sum_{s \in \Omega(0,0)} f(s) \\ &= \frac{1}{3^{\ell-1}} \sum_{\substack{u_0, u_1, u_2 \\ u_0 + u_1 + u_2 = \ell}} \binom{\ell-1}{u_0-1} \binom{\ell-u_0}{u_1} (g_0(u_0) + g_1(u_1) + g_2(u_2)). \end{aligned}$$

Of course, the same argument shows that

$$\begin{aligned} f_{(i,1)} &= \frac{1}{3^{\ell-1}} \sum_{s \in \Omega(0,1)} f(s) \\ &= \frac{1}{3^{\ell-1}} \sum_{\substack{u_0, u_1, u_2 \\ u_0 + u_1 + u_2 = \ell}} \binom{\ell-1}{u_1-1} \binom{\ell-u_1}{u_2} (g_0(u_0) + g_1(u_1) + g_2(u_2)) \end{aligned}$$

and

$$\begin{aligned} f_{(i,2)} &= \frac{1}{3^{\ell-1}} \sum_{s \in \Omega(0,2)} f(s) \\ &= \frac{1}{3^{\ell-1}} \sum_{\substack{u_0, u_1, u_2 \\ u_0 + u_1 + u_2 = \ell}} \binom{\ell-1}{u_2-1} \binom{\ell-u_2}{u_0} (g_0(u_0) + g_1(u_1) + g_2(u_2)). \end{aligned}$$

So, if $1 \leq k \leq 2$, we have that

$$\begin{aligned} w_{k3^i} &= 3^{-\ell/2} \sum_{\substack{u_0, u_1, u_2 \\ u_0 + u_1 + u_2 = \ell}} \left\{ \binom{\ell-1}{u_0-1} \binom{\ell-u_0}{u_1} + r^k \binom{\ell-1}{u_1-1} \binom{\ell-u_1}{u_2} \right. \\ &\quad \left. + r^{2k} \binom{\ell-1}{u_2-1} \binom{\ell-u_2}{u_0} \right\} (g_0(u_0) + g_1(u_1) + g_2(u_2)). \end{aligned}$$

In the general case, we find

$$w_{kn^i} = n^{-\frac{\ell}{2}} \sum_{\substack{u_0, \dots, u_{n-1} \\ u_0 + \dots + u_{n-1} = \ell}} \alpha_{u_0 \dots u_{n-1}}^k \sum_{i=0}^{n-1} g_p(u_p)$$

with

$$\alpha_{u_0 \dots u_{n-1}}^k = \sum_{i=0}^{n-1} r^{ki} \binom{\ell-1}{u_i-1} \binom{\ell-u_i}{u_{i+1}} \dots \binom{\ell-u_i-u_{i+1}-\dots-u_{i+n-3}}{u_{i+n-2}},$$

where all coefficients are modulo ℓ .

On the other hand, note that

$$w_0 = n^{-\frac{\ell}{2}} \sum_{s \in \Omega} f(s) = n^{-\frac{\ell}{2}} \sum_{\substack{u_0, \dots, u_{n-1} \\ u_0 + \dots + u_{n-1} = \ell}} \sum_{\substack{s \in \Omega \\ \forall i: u_i(s) = u_i}} f(s).$$

Since f is a unitation function,

$$w_0 = n^{-\frac{\ell}{2}} \sum_{\substack{u_0, \dots, u_{n-1} \\ u_0 + \dots + u_{n-1} = \ell}} \binom{\ell}{u_0} \binom{\ell-u_0}{u_1} \dots \binom{\ell-u_0-\dots-u_{n-3}}{u_{n-2}} \sum_{i=0}^{n-1} g_i(u_i).$$

The normalized epistasis of f is thus finally given by

$$\varepsilon_{n,\ell}^*(f) = 1 - \frac{|w_0|^2 + \ell \sum_{k=1}^{n-1} |w_k|^2}{\sum_{i=0}^{n-1} |w_i|^2},$$

with coefficients as above.

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