Multary epistasis

M. T. Iglesias C. Vidal* D. Suys A. Verschoren†

Abstract

In this note, we introduce and study the notion of normalized epistasis of a fitness function over not necessary binary alphabets, as an indicator of its GA-hardness. Fitness functions with minimal and maximal normalized epistasis are explicitly described.

Introduction

The classical genetic algorithm (GA) starts from a positive real-valued function f on $\Omega = \{0,1\}^\ell$ (the set of all length ℓ strings $s = s_{\ell-1} \dots s_0$), whose maximum (or minimum) we want to find. It has long been understood (in particular through examples given in [3, et al]) that linkage between bits may make it hard for the GA to find the maximum of f. In [5] Rawlins compares this phenomenon to the analogous 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. [6]. 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 thus speaks of *minimal* (or *zero*) *epistasis*, when every bit is independent of any other one, i.e., if the fitness function f may be given as

$$f(s_{\ell-1} \dots s_0) = \sum_{i=0}^{\ell-1} g(i, s_i).$$

*Supported by a University of La Coruña project.

†Research supported by the N.F.W.O. and the European H.C.M.-project.

Received by the editors February 2000.

Communicated by Y. Félix.

1991 *Mathematics Subject Classification :* 68Q25, 68T20, 68R05.

Key words and phrases : Epistasis, Genetic algorithm, optimisation.

At the other extreme, we have *maximal epistasis*, if no proper subset of genes is independent of any other gene, and this situation amounts to f essentially being a random function.

Any reasonable quantification of the previous ideas should associate to every fitness function f on Ω a positive real number $\varepsilon(f)$ in such a way that $\varepsilon(f) = 0$ corresponds to minimal epistasis. Moreover, since for any fitness function f and any real number r both f and rf share the same "linked" bits, one should have $\varepsilon(rf) = \varepsilon(f)$, thus leading to a notion of *normalized epistasis*. Extending ideas due to Davidor [1], normalized epistasis was introduced and studied in [7, 8, 9, 10], and shown to give useful indications concerning the GA-hardness of certain fitness functions, due to epistatic phenomena.

As its title indicates, in this note, we aim to study epistasis over not necessarily binary alphabets. We will not go into motivating the use of these, as this falls outside of the scope of the present text, instead referring to [2] for example (from which we also borrowed the term "multary" for alphabets which are not necessarily binary). Let us just mention that, although binaring encodings are "standard" in the GA context, sometimes it is much more natural to use a different type of encoding, in particular when characteristics of data are characterized by arbitrary integers, for example, or when a quick and intuitive interpretation of the chains representing data is required.

In the first part of this note, we introduce and study the notion of normalized epistasis $\varepsilon^*(f)$ for a fitness function f acting on strings over a multary alphabet and derive its main properties. In the second part, we consider the extreme values of $\varepsilon^*(f)$ and relate this to minimal and maximal epistasis.

1 Epistasis

1.1. *Throughout this text, we will work over a fixed alphabet A of cardinality n, which we usually identify with the set of integers $\{0, \ldots, n-1\}$. The set A^ℓ of length ℓ strings $s = s_{\ell-1} \ldots s_0$ over A will be denoted by Ω. Let $\mathbb{R}_+$ be the set of all positive real numbers.* Fitness functions *are maps $f : \Omega \to \mathbb{R}_+$ (which we want to optimize). Following 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 $0 \leq i \leq \ell - 1$ and $a \in A$ by

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

the average fitness over $P(a, i)$, the sub-population consisting of all strings $s_{\ell-1} \ldots s_0 \in P$ with $s_i = a$. The excess allele value $E_P(i, a)$ is defined to be $f_{P(i,a)} - f_P$ and the excess genic value as $E_P(s) = \sum_{i=0}^{\ell-1} E_P(i, s_i)$. The genic value of $s \in P$ (the "expected" fitness value) is finally given by $f'_P(s) = E_P(s) + f_P(s)$, and the epistasis *of s (with respect to P) by $\varepsilon_P(s) = f(s) - f'_P(s)$.*

A straightforward calculation shows that this definition may be rewritten as

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

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

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

In this case, the global epistasis *of* f *is defined to be*

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

1.2. *As in [7, 9, 10], the previous definition may be rewritten in a more elegant way. Indeed, consider*

$$\mathbf{e} = \begin{pmatrix} \varepsilon(0\ldots 00) \\ \varepsilon(0\ldots 01) \\ \vdots \\ \varepsilon((n-1)^{(\ell)}) \end{pmatrix} \quad \textit{resp.}\ \mathbf{f} = \begin{pmatrix} f(0\ldots 00) \\ f(0\ldots 01) \\ \vdots \\ f((n-1)^{(\ell)}) \end{pmatrix},$$

where $(n-1)^{(\ell)}$ *is the length* ℓ *string* $(n-1)\ldots(n-1)$*. We will also use the notation* $f_0, \ldots, f_{n^\ell-1}$ *for* $f(0\ldots 00), \ldots, f((n-1)^{(\ell-1)})$*, so*

$$\mathbf{f} = \begin{pmatrix} f_0 \\ \vdots \\ f_{n^\ell-1} \end{pmatrix}.$$

For any $0 \le i, j \le n^\ell - 1$*, let us put*

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

where d_{ij} *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.*

Denote by $\mathbf{E}_\ell$ *the* n^ℓ*-dimensional rational matrix* (e_{ij})*. It is easy to see that we then have*

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

We thus obtain that the global epistasis of f *is given by*

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

1.3. *Since for any positive real number* $r \in \mathbb{R}$ *and any fitness function* f *we have that* $\varepsilon(rf) = r\varepsilon(f)$*, we obviously cannot use global epistasis directly as a measure of GA hardness. In order to remedy this, as in [7, 8], we define the* normalized epistasis *of the fitness function* f *as*

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

where $\mathbf{F}_\ell = \mathbf{I}_\ell - \mathbf{E}_\ell$ *is an orthogonal projection (being idempotent and symmetric). It follows that* $0 \le \varepsilon_\ell^*(f) \le 1$*, for any fitness function* f*.*

1.4. *As pointed out in [8, 9, 10], normalized epistasis may be used as an indicator of GA-hardness. Let us work in the binary case, for a moment and consider the following generalization of Forrest and Mitchell's Royal Road functions, cf. [3, 4]. For any positive integers* $m \leq n$ *and* $0 \leq i \leq 2^{n-m} - 1$, *define length* 2^n *schemata*

$$H_i^{n,m} = *^{(2^m i)} 1^{(2^m)} *^{(2^n - 2^m(i+1))},$$

where for any $a \in \{0, 1, *\}$, *we denote by* $a^{(p)}$ *the length* p *string* $a \ldots a$. *Define the fitness function* R_m^n *by letting* $R_m^n(s) = 2^m c_{n,m}(s)$, *where for any length* 2^n *string* s, *we denote by* $c_{n,m}(s)$ *the number of schemata* $H_i^{n,m}$ *to which* s *belongs. Clearly,* R_0^n *is linear (it counts the number of 1's in any length* 2^n *string), whereas for fixed* n, *it appears that for increasing* m *the functions* R_m^n *have corresponding increasing normalized epistasis. In particular,* R_n^n *is the "Dirac function"* d_n *with single peak* 2^n *at* $1 \ldots 1$.

As a typical example, let us work with strings of length 64 ($n = 6$*) and population size 128. As a measure of GA-hardness, we experimentally calculated the average number* $G(f)$ *of generations needed to obtain that :*

- *at least one member of the population has maximum fitness* μ *(the string* $1^{(64)}$*);*
- *the average fitness of the population is higher than* $0.9 \times \mu$*;*
- $\frac{\textit{standard deviation}}{\textit{average}} \leq 0.05$.

we then obtained :

f	$G(f)$	$\varepsilon_\ell^*(f)$
R_0^6	*37*	*0.00*
R_1^6	*61*	*0.03*
R_2^6	*99*	*0.35*
R_3^6	*920*	*0.94*
R_4^6	> 1500	*0.99*
R_5^6	> 1500	*1.00*
R_6^6	> 1500	*1.00*

For other values of n *and* m, *the functions* R_m^n *behave similarly – we refer to [4] for details, as well as theoretical and experimental results.*

2 Eigenvalues and eigenspaces

2.1. *Let us fix a positive integer* ℓ. *With notations as before, consider the integer matrix* $\mathbf{G}_\ell = n^\ell \mathbf{E}_\ell$, *i.e.,* $\mathbf{G}_\ell = (g_{ij}^\ell)$, *with* $g_{ij}^\ell = (n-1)\ell + 1 - nd_{ij}$ *for every* $0 \leq i, j \leq n^\ell - 1$. *If no ambiguity arises, we just write* g_{ij} *for* g_{ij}^ℓ.

The following result appears to be very useful :

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

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

where, for any positive integer k, the n^k-dimensional matrix $\mathbf{U}_k$ is given by

$$\mathbf{U}_k = \begin{pmatrix} 1 & \cdots & 1 \\ \vdots & \ddots & \vdots \\ 1 & \cdots & 1 \end{pmatrix}.$$

Proof. The length ℓ words over the alphabet A (with $|A| = n$) may be subdivided into n subclasses, each of these determined by the "bit" at position ℓ. This subdivision allows us to view the matrix $\mathbf{G}_\ell$ as composed of n^2 submatrices $\mathbf{G}_{pq}$, say

$$\mathbf{G}_\ell = \begin{pmatrix} \mathbf{G}_{00} & \cdots & \mathbf{G}_{0,n-1} \\ \vdots & \ddots & \vdots \\ \mathbf{G}_{n-1,0} & \cdots & \mathbf{G}_{n-1,n-1} \end{pmatrix},$$

with $\mathbf{G}_{pq} = (g_{ij}^\ell)$, where i resp. j varies through the elements in A^ℓ with p resp. q in bit-position ℓ.

For any $0 \le i, j < n^\ell$, denote by d_{ij}^ℓ the Hamming distance between the length ℓ n-ary representations of i and j and by $d_{ij}^{\ell-1}$ the Hamming distance between the length ℓ-1 vectors obtained from the previous ones by eliminating the ℓ-th bit. For example, since the ternary representation of 23 resp. 19 is 212 resp. 201, we have $d_{23,19}^3 = d_{23,19}^2 = 2$. As the ternary representation of 13 is 111, we also have $d_{13,19}^3 = 2$, while $d_{13,19}^2 = 1$.

For every $0 \le p \le n-1$, we have $\mathbf{G}_{pp} = \mathbf{G}_{\ell-1} + (n-1)\mathbf{U}_{\ell-1}$. Indeed,

$$\begin{aligned} \mathbf{G}_{pp} &= (g_{ij}^\ell) = ((n-1)\ell + 1 - nd_{ij}^\ell) \\ &= ((n-1)(\ell-1) + 1 - nd_{ij}^\ell + (n-1)) \\ &= ((n-1)(\ell-1) + 1 - nd_{ij}^{\ell-1} + (n-1)) \\ &= \mathbf{G}_{\ell-1} + (n-1)\mathbf{U}_{\ell-1}, \end{aligned}$$

since, in this case, we always have $d_{ij}^\ell = d_{ij}^{\ell-1}$.

Outside of the diagonal, i.e., with $0 \le p \ne q \le n-1$, we have

$$\begin{aligned} \mathbf{G}_{pq} &= (g_{ij}^\ell) = ((n-1)\ell + 1 - nd_{ij}^\ell) \\ &= ((n-1)(\ell-1) + 1 - nd_{ij}^\ell + (n-1)) \\ &= ((n-1)(\ell-1) + 1 - n(d_{ij}^{\ell-1} + 1) + (n-1)) \\ &= \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1}, \end{aligned}$$

since, in this case, we always have $d_{ij}^\ell = d_{ij}^{\ell-1} + 1$. This finishes the proof. ∎

As a consequence, let us mention :

Corollary. 2.3. *For any positive integer ℓ, we have $\mathbf{G}_\ell^2 = n^\ell \mathbf{G}_\ell$.*

Proof. The statement obviously holds true for $\ell = 0$ resp. $\ell = 1$, where $\mathbf{G}_0 = (1)$ resp. $\mathbf{G}_1 = n\mathbf{I}_n$ ($\mathbf{I}_n$ denoting the n-dimensional identity matrix). The general case follows from a straightforward induction argument, using the previous result. ∎

Note that this result implies that the eigenvalues of $\mathbf{G}_\ell$ are 0 and n^ℓ. Indeed, as $\mathbf{G}_\ell$ is a symmetric real matrix, its eigenvalues are well known to be real. On the other hand, if $\mathbf{v}$ is an eigenvector of $\mathbf{G}_\ell$, say with eigenvalue λ, i.e., $\mathbf{G}_\ell\mathbf{v} = \mathbf{v}\lambda$, then

$$n^\ell\lambda\mathbf{v} = n^\ell\mathbf{G}_\ell\mathbf{v} = \mathbf{G}_\ell^2\mathbf{v} = \lambda^2\mathbf{v}.$$

So, $\lambda = 0$ or $\lambda = n^\ell$, as we claimed.

. *From the identity* $\mathbf{G}_\ell = n^\ell\mathbf{G}_\ell$, *it also follows :*

Corollary. 2.4. *For any positive integer ℓ, the matrix $\mathbf{E}_\ell$ is idempotent. In particular, $\mathbf{E}_\ell$ has eigenvalues 0 and 1.*

In order to determine the eigenspaces of $\mathbf{G}_\ell$ (and $\mathbf{E}_\ell$), let us first calculate its rank.

Lemma. 2.5. *For any positive integer ℓ, we have*

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

Proof. Let us again argue by induction on ℓ. The assertion holds true for $\ell = 1$. On the other hand, applying 2.2, elementary row and column operations reduce $\mathbf{G}_\ell$ to the form

$$\begin{pmatrix} n\mathbf{G}_{\ell-1} & 0 & \cdots & 0 \\ 0 & \mathbf{U}_{\ell-1} & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \mathbf{U}_{\ell-1} \end{pmatrix}.$$

This yields that

$$\begin{aligned} rk(\mathbf{G}_\ell) &= rk(\mathbf{G}_{\ell-1}) + (n-1)rk(\mathbf{U}_{\ell-1}) \\ &= ((n-1)(\ell-1)+1) + (n-1) = (n-1)\ell + 1, \end{aligned}$$

which proves the assertion. ∎

2.6. *Let us denote by V_0^ℓ resp. V_1^ℓ the eigenspace in $\mathbb{R}^{n^\ell}$ corresponding to the eigenvalue 0 resp. n^ℓ of $\mathbf{G}_\ell$ (or, equivalently, the eigenvalue 0 resp. 1 of $\mathbf{E}_\ell$). Then $\mathbb{R}^{n^\ell} = V_0^\ell \oplus V_1^\ell$, and, as $V_0^\ell = Ker(\mathbf{G}_\ell)$ resp. $V_1^\ell = Im(\mathbf{G}_\ell)$, the previous result yields that*

$$dim(V_0^\ell) = n^\ell - (n-1)\ell - 1$$

resp.

$$dim(V_1^\ell) = (n-1)\ell + 1.$$

An explicit orthogonal basis for V_1^ℓ may be constructed as follows. Start from $\mathbf{v}_0^0 = 1$, and suppose we already constructed a subset

$$\{\mathbf{v}_0^{\ell-1}, \ldots, \mathbf{v}_{(n-1)(\ell-1)}^{\ell-1}\} \subseteq \mathbb{R}^{n^{\ell-1}}.$$

We construct a new subset

$$\{\mathbf{v}_0^\ell, \ldots, \mathbf{v}_{(n-1)\ell}^\ell\} \subseteq \mathbb{R}^{n^\ell}$$

where

$$\mathbf{v}_k^\ell = \begin{pmatrix} \mathbf{v}_k^{\ell-1} \\ \vdots \\ \mathbf{v}_k^{\ell-1} \end{pmatrix}$$

for all $0 \le k \le (n-1)(\ell-1)$ *and where* $\mathbf{v}^\ell_{(n-1)(\ell-1)+1}, \mathbf{v}^\ell_{(n-1)(\ell-1)+2}, \dots, \mathbf{v}^\ell_{(n-1)\ell}$ *are given by*

$$\begin{pmatrix} \mathbf{e}_{\ell-1} \\ -\mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix}, \begin{pmatrix} \mathbf{e}_{\ell-1} \\ \mathbf{e}_{\ell-1} \\ -2\mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix}, \dots, \begin{pmatrix} \mathbf{e}_{\ell-1} \\ \mathbf{e}_{\ell-1} \\ \vdots \\ \mathbf{e}_{\ell-1} \\ \mathbf{e}_{\ell-1} \\ -(n-1)\mathbf{e}_{\ell-1} \end{pmatrix},$$

with

$$\mathbf{e}_{\ell-1} = \begin{pmatrix} 1 \\ \vdots \\ 1 \end{pmatrix} \ \textit{resp.}\ \mathbf{0}_{\ell-1} = \begin{pmatrix} 0 \\ \vdots \\ 0 \end{pmatrix}$$

within $\mathbb{R}^{n^{\ell-1}}$.

As an example, if $n = 3$ *and* $\ell = 1$*, then*

$$\mathbf{v}_0^1 = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}, \mathbf{v}_1^1 = \begin{pmatrix} 1 \\ -1 \\ 0 \end{pmatrix}, \mathbf{v}_2^1 = \begin{pmatrix} 1 \\ 1 \\ -2 \end{pmatrix}$$

so, for $n = 3$ *and* $\ell = 2$*, we obtain*

$$\mathbf{v}_0^2 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \mathbf{v}_1^2 = \begin{pmatrix} 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \\ 1 \\ -1 \\ 0 \end{pmatrix}, \mathbf{v}_2^2 = \begin{pmatrix} 1 \\ 1 \\ -2 \\ 1 \\ 1 \\ -2 \\ 1 \\ 1 \\ -2 \end{pmatrix}, \mathbf{v}_3^2 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ -1 \\ -1 \\ -1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \mathbf{v}_4^2 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ 1 \\ -2 \\ -2 \\ -2 \end{pmatrix}.$$

We may now prove :

Proposition. 2.7. *With the previous notations, for every positive integer* ℓ*, the set*

$$\{\mathbf{v}_0^\ell, \dots, \mathbf{v}_{(n-1)\ell}^\ell\}$$

is an orthogonal basis for V_1^ℓ.

Proof. For $\ell = 0$, the statement is obvious. Suppose the assertion holds true for strings of length $0, \dots, \ell-1$ and let us prove it for strings of length ℓ. In this case, if $0 \le k \ne k' \le (n-1)(\ell-1)$, then the induction hypothesis implies that ${}^t\mathbf{v}_k^\ell \mathbf{v}_{k'}^\ell = 0$. On the other hand, if

$$0 \le k \le (n-1)(\ell-1) < k' \le (n-1)\ell,$$

then

$$
{}^t\mathbf{v}_k^\ell \mathbf{v}_{k'}^\ell = ({}^t\mathbf{v}_k^{\ell-1}, \ldots, {}^t\mathbf{v}_k^{\ell-1}) \begin{pmatrix} \mathbf{e}_{\ell-1} \\ \vdots \\ \mathbf{e}_{\ell-1} \\ -i\mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix} = i\,{}^t\mathbf{v}_k^{\ell-1}\mathbf{e}_{\ell-1} - i\,{}^t\mathbf{v}_k^{\ell-1}\mathbf{e}_{\ell-1} = 0.
$$

Finally, if $(n-1)(\ell-1)+1 \leq k \neq k' \leq (n-1)\ell$, then

$$
{}^t\mathbf{v}_k^\ell \mathbf{v}_{k'}^\ell = ({}^t\mathbf{e}_{\ell-1}, \ldots, {}^t\mathbf{e}_{\ell-1}, -i\,{}^t\mathbf{e}_{\ell-1}, {}^t\mathbf{0}_{\ell-1}, \ldots, {}^t\mathbf{0}_{\ell-1}) \begin{pmatrix} \mathbf{e}_{\ell-1} \\ \vdots \\ \mathbf{e}_{\ell-1} \\ -j\mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix} = 0.
$$

Since the vectors $\mathbf{v}_0^\ell, \ldots, \mathbf{v}_{(n-1)\ell}^\ell$ are obviously linearly independent, it thus suffices to verify that they belong to V_1^ℓ, as we have seen that $dim(V_1^\ell) = (n-1)\ell + 1$.

Let us again argue by induction on ℓ. For $\ell = 0$, the statement is obvious, so let us assume it to hold true for length $0, \ldots, \ell - 1$ and prove it for length ℓ. First, if $0 \leq k \leq (n-1)(\ell-1)$, then

$$
\begin{aligned}
\mathbf{G}_\ell \mathbf{v}_k^\ell &= \begin{pmatrix} \mathbf{G}_{\ell-1} + (n-1)\mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} \\ \vdots & \ddots & \vdots \\ \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{\ell-1} + (n-1)\mathbf{U}_{\ell-1} \end{pmatrix} \begin{pmatrix} \mathbf{v}_k^{\ell-1} \\ \vdots \\ \mathbf{v}_k^{\ell-1} \end{pmatrix} \\
&= \begin{pmatrix} n\mathbf{G}_{\ell-1}\mathbf{v}_k^{\ell-1} \\ \vdots \\ n\mathbf{G}_{\ell-1}\mathbf{v}_k^{\ell-1} \end{pmatrix} = n.n^{\ell-1} \begin{pmatrix} \mathbf{v}_k^{\ell-1} \\ \vdots \\ \mathbf{v}_k^{\ell-1} \end{pmatrix} = n^\ell \mathbf{v}_k^\ell.
\end{aligned}
$$

On the other hand, if $k = (n-1)(\ell-1)+i$ with $1 \leq i \leq n-1$, then

$$\mathbf{G}_\ell \mathbf{v}_k^\ell = \begin{pmatrix} \mathbf{G}_{\ell-1}+(n-1)\mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{\ell-1}-\mathbf{U}_{\ell-1} \\ \vdots & \ddots & \vdots \\ \mathbf{G}_{\ell-1}-\mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{\ell-1}+(n-1)\mathbf{U}_{\ell-1} \end{pmatrix} \begin{pmatrix} \mathbf{e}_{\ell-1} \\ \vdots \\ \mathbf{e}_{\ell-1} \\ -i\mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix}$$

$$= n \begin{pmatrix} \mathbf{U}_{\ell-1}\mathbf{e}_{\ell-1} \\ \vdots \\ \mathbf{U}_{\ell-1}\mathbf{e}_{\ell-1} \\ -i\mathbf{U}_{\ell-1}\mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix} = n.n^{\ell-1} \begin{pmatrix} \mathbf{e}_{\ell-1} \\ \vdots \\ \mathbf{e}_{\ell-1} \\ -i\mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix} = n^\ell \mathbf{v}_k^\ell.$$

This finishes the proof. ∎

2.8. *We have already pointed out above, that $0 \leq \varepsilon_\ell^*(f) \leq 1$. ¿From the previous remarks, it is now clear that $\varepsilon_\ell^*(f) = 0$ resp. $\varepsilon_\ell^*(f) = 1$ exactly when $\mathbf{f} \in V_1^\ell$ resp. $\mathbf{f} \in V_0^\ell$. As an example, if $n = 3$ and $\ell = 2$, then it thus follows that $\mathbf{f} \in V_1^\ell$ if and only if it belongs to the vector space generated by the vectors*

$$\begin{pmatrix} 1\\1\\1\\1\\1\\1\\1\\1\\1 \end{pmatrix}, \begin{pmatrix} 1\\-1\\0\\1\\-1\\0\\1\\-1\\0 \end{pmatrix}, \begin{pmatrix} 1\\1\\-2\\1\\1\\-2\\1\\1\\-2 \end{pmatrix}, \begin{pmatrix} 1\\1\\1\\-1\\-1\\-1\\0\\0\\0 \end{pmatrix}, \begin{pmatrix} 1\\1\\1\\1\\1\\1\\-2\\-2\\-2 \end{pmatrix}.$$

This is easily seen to be equivalent to

$$f_{01}+f_{02}+f_{10}+f_{12}+f_{20}+f_{21} = 2(f_{00}+f_{11}+f_{22}).$$

3 Minimal epistasis

It is clear that the minimal resp. maximal values of $\varepsilon_\ell^*(f)$ correspond to the maximal resp. minimal values of

$$\gamma_\ell(f) = {}^t\mathbf{f}\mathbf{G}_\ell\mathbf{f},$$

with $||\mathbf{f}|| = 1$. In particular, $0 \leq \gamma_\ell(f) \leq n^\ell$.

In the next sections, we will take a closer look at these extreme values and connect them to Rawlins' notion of minimal and maximal epistasis.

3.1. *Let us first point out that the theoretical minimal value $\varepsilon_\ell^*(f) = 0$ (or, equivalently, the maximal value $\gamma_\ell(f) = n^\ell$) may actually be reached. Indeed, if $\ell = 1$, then dim$(V_1^1) = n$, so $V_1^1 = \mathbb{R}^n$, and any $\mathbf{f} \in \mathbb{R}^n$ with $||\mathbf{f}|| = 1$ satisfies*

$$\gamma_1(f) = {}^t\mathbf{f}\mathbf{G}_\ell\mathbf{f} = (f_0 \dots f_{n-1}) \begin{pmatrix} n & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & n \end{pmatrix} \begin{pmatrix} f_0 \\ \vdots \\ f_{n-1} \end{pmatrix} = n\sum_{i=0}^{n-1} f_i^2 = n.$$

In the general case, i.e., when $\ell > 1$, we will need the following result :

Lemma. 3.2. *For any positive integer ℓ, we have*

$$\sum_{i,j} g_{ij}^\ell = n^{2\ell}.$$

Proof. Let us apply induction on ℓ. For $\ell = 1$, we have $\mathbf{G}_1 = n\mathbf{I}_n$, so the result is obviously correct. Assume it holds true for length $1, \dots, \ell - 1$ and let us prove it for length ℓ. To realize this, it suffices to apply 2.2, which easily yields that

$$\sum_{i,j} g_{ij}^\ell = n^2 \sum_{i,j} g_{ij}^{\ell-1} = n^2.n^{2(\ell-1)} = n^{2\ell}.$$

This proves our assertion. ∎

3.3. *Consider the vector*

$$\mathbf{f}' = \begin{pmatrix} \mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \\ \mathbf{e}_{\ell-1} \end{pmatrix}$$

and put $\mathbf{f} = \mathbf{f}'/||\mathbf{f}'||$, then we claim that $\varepsilon_\ell^*(f) = 0$ (which proves that minimal normalized epistasis may always be realized). Indeed,

$$\begin{aligned}
\gamma_\ell(f) &= {}^t\mathbf{f}\mathbf{G}_\ell\mathbf{f} = \frac{1}{||\mathbf{f}'||^2}{}^t\mathbf{f}'\mathbf{G}_\ell\mathbf{f}' \\
&= \frac{1}{2n^{\ell-1}}{}^t\mathbf{f}' \begin{pmatrix} \mathbf{G}_{\ell-1} + (n-1)\mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} \\ \vdots & \ddots & \vdots \\ \mathbf{G}_{\ell-1} - \mathbf{U}_{\ell-1} & \cdots & \mathbf{G}_{\ell-1} + (n-1)\mathbf{U}_{\ell-1} \end{pmatrix} \mathbf{f}' \\
&= 2\frac{1}{2n^{\ell-1}}{}^t\mathbf{e}_{\ell-1}(2\mathbf{G}_{\ell-1} + (n-2)\mathbf{U}_{\ell-1})\mathbf{e}_{\ell-1} \\
&= \frac{1}{n^{\ell-1}}(2\sum_{i,j} g_{ij}^{\ell-1} + (n-2)\sum_{i,j} u_{ij}^{\ell-1}) \\
&= \frac{1}{n^{\ell-1}}(2n^{2(\ell-1)} + (n-2)n^{2(\ell-1)}) = n^\ell.
\end{aligned}$$

3.4. *It has been proved in [9], that, over a binary alphabet, a fitness function f has $\varepsilon^*(f) = 0$ if and only if f has minimal epistasis in the sense of [5], i.e., if f may be written in the form*

$$f(s_{\ell-1} \dots s_0) = \sum_{i=0}^{\ell-1} g(i, s_i).$$

In order to extend this result to a cardinality n alphabet, let us define for any $0 \leq i \leq \ell - 1$ and $1 \leq j \leq n-1$ the map

$$h_{ij}^{\ell} \ : \Omega \to \mathbb{R} \ : s = s_{\ell-1} \dots s_0 \mapsto \begin{cases} 1 & \textit{if} \quad s_i = j \\ 0 & \textit{if} \quad s_i \neq j \end{cases} .$$

Denote by $\mathbf{h}_{ij}^{\ell}$ the corresponding vector in $\mathbb{R}^{n^{\ell}}$. Clearly, for any $0 \leq i \leq \ell - 2$, we have

$$\mathbf{h}_{ij}^{\ell} = \begin{pmatrix} \mathbf{h}_{ij}^{\ell-1} \\ \vdots \\ \mathbf{h}_{ij}^{\ell-1} \end{pmatrix}$$

whereas,

$$\mathbf{h}_{\ell-1,1}^{\ell} = \begin{pmatrix} \mathbf{0}_{\ell-1} \\ \mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix}, \mathbf{h}_{\ell-1,2}^{\ell} = \begin{pmatrix} \mathbf{0}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \mathbf{e}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \end{pmatrix}, \dots, \mathbf{h}_{\ell-1,\ell-1}^{\ell} = \begin{pmatrix} \mathbf{0}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \vdots \\ \mathbf{0}_{\ell-1} \\ \mathbf{0}_{\ell-1} \\ \mathbf{e}_{\ell-1} \end{pmatrix} \in \mathbb{R}^{n^{\ell}}.$$

Lemma. 3.5. *The set*

$$\{\mathbf{e}_{\ell}, \mathbf{h}_{ij}^{\ell}; 0 \leq i \leq \ell - 1, 1 \leq j \leq n-1\}$$

is linearly independent.

Proof. Suppose that

$$\sum_{i=0}^{\ell-1} \alpha_{i1} \mathbf{h}_{i1}^{\ell} + \ldots + \sum_{i=0}^{\ell-1} \alpha_{i,n-1} \mathbf{h}_{i,n-1}^{\ell} + \beta \mathbf{e}_{\ell} = \mathbf{0}_{\ell},$$

and denote by g the corresponding real-valued function

$$\sum_{i=1}^{\ell-1} \alpha_{i1} h_{i1}^{\ell} + \ldots + \sum_{i=1}^{\ell-1} \alpha_{i,n-1} h_{i,n-1}^{\ell} + \beta e_{\ell}$$

on Ω. We then clearly have $\beta = g(0) = 0$. On the other hand, for every $1 \leq j \leq n-1$ and $0 \leq i \leq \ell - 1$, we have

$$0 = g(jn^i) = \sum_{k=0}^{\ell-1} \alpha_{kj} h_{kj}^{\ell}(jn^i) + \beta = \alpha_{ij}.$$

This proves the assertion. ∎

Since a reasoning similar to that in 2.7 shows that the vectors $\mathbf{h}_{ij}^{\ell}$ and $\mathbf{e}_{\ell}$ belong to V_1^{ℓ}, it thus follows that they actually form a *basis* for V_1^{ℓ}.

We are now ready to prove :

Theorem. 3.6. *For any fitness function f on Ω, the following assertions are equivalent :*

1. *f has minimal epistasis, i.e., $f = \sum_{i=0}^{\ell-1} g_i$ for some fitness functions g_i, which only depend on the i-th bit;*
2. *$\varepsilon^*(f) = 0$.*

Proof. Clearly, if f has minimal epistasis, i.e., if $f = \sum_{i=0}^{\ell-1} g_i$, where g_i only depends upon the i-th bit, then $\mathbf{f} \in V_1^\ell$, hence $\varepsilon^*(f) = 0$. Indeed, it suffices to verify this for each of the $\mathbf{g}_i$. Now, if we let a_{ij} denote the common value of all $g_i(s)$ with i-th bit equal to j (with $1 \leq j \leq n-1$), then

$$g_i = \sum_{j=1}^{n-1} a_{ij} h_{ij}^\ell + a_{i0}(e_\ell - h_{i1}^\ell - \ldots - h_{i,n-1}^\ell),$$

so $\mathbf{g}_i \in <\mathbf{h}_{ij}^\ell, \mathbf{e}_\ell >= V_1^\ell$.

Conversely, if $\mathbf{f} \in V_1^\ell$, then

$$\mathbf{f} = \sum_{i,j} \alpha_{ij}\mathbf{h}_{ij}^\ell + \beta\mathbf{e}_\ell = \sum_{i=0}^{\ell-1}(\sum_{j=1}^{n-1} \alpha_{ij}\mathbf{h}_{ij}^\ell) + \beta\mathbf{e}_\ell = \sum_{i=0}^{\ell-1} \mathbf{g}_i,$$

where

$$\mathbf{g}_0 = (\alpha_{01} + \beta)\mathbf{h}_{01}^\ell + \beta(\mathbf{e}_\ell - \mathbf{h}_{01}^\ell) + \sum_{j=2}^{n-1} \alpha_{02}\mathbf{h}_{02}^\ell$$

and

$$\mathbf{g}_i = \sum_{j=1}^{n-1} \alpha_{ij}\mathbf{h}_{ij}^\ell \text{ with } 1 \leq i \leq \ell - 1.$$

∎

4 Maximal epistasis

4.1. *In this section, we will analyze the maximal value of $\varepsilon_\ell^*(f)$. We have already pointed out that $\varepsilon_\ell^*(f) \leq 1$. Moreover, for any $\mathbf{f} \in V_0^\ell$ this maximum value is actually reached. However, in the present context, one has to impose the extra restriction that all coordinates of $\mathbf{f}$ be positive, as $\mathbf{f}$ should correspond to a (positively valued!) fitness function on Ω. It appears that under this condition, the maximal value that $\varepsilon_\ell^*(f)$ may reach is $1 - \frac{1}{n^{\ell-1}}$. Equivalently : the minimal value of $\gamma_\ell(f)$ with $||\mathbf{f}|| = 1$ is n.*

The main purpose of this section is proving this result. In the next one, we give a precise description of those fitness functions which realize this maximum value.

4.2. *Let us first point out that the extreme value $\gamma_\ell(n) = n$ may actually be reached. Indeed, consider the vector $\mathbf{f} \in \mathbb{R}^{n^\ell}$, given by*

$${}^t\mathbf{f} = (\alpha, 0, \ldots, 0, \alpha, 0, \ldots, 0, \alpha),$$

where $\alpha = \sqrt{n}/n$ *appears as* $i\frac{n^\ell-1}{n-1}$*-th coordinate, for* $0 \leq i \leq n-1$. *Obviously* $||\mathbf{f}|| = 1$. *Moreover, with* $m = \frac{n^\ell-1}{n-1}$, *we have*

$$\begin{aligned}
\gamma_\ell(f) &= {}^t\mathbf{f}\mathbf{G}_\ell\mathbf{f} \\
&= \alpha^2((g_{00} + g_{0m} + \ldots + g_{0,n^\ell-1}) + (g_{m0} + \ldots + g_{m,n^\ell-1}) \\
&\quad + \ldots + (g_{n^\ell-1,0} + \ldots + g_{n^\ell-1,n^\ell-1})) \\
&= \frac{1}{n}((g_{00} + g_{mm} + \ldots + g_{n^\ell-1,n^\ell-1}) + 2(g_{0m} + \ldots + g_{(n-2)m,m})) \\
&= \frac{1}{n}(ng_{00} + 2\sum_{i<j} g_{im,jm}).
\end{aligned}$$

Since each of the $g_{im,jm}$ *has the same value* $(n-1)\ell + 1 - n\ell$, *it thus easily follows that* $\gamma_l(f) = n$, *as claimed.*

Theorem. 4.3. *For any positive integer* ℓ *and any positive valued fitness function* f *with* $||\mathbf{f}|| = 1$, *we have*

$$\varepsilon_\ell^*(f) \leq 1 - \frac{1}{n^{\ell-1}}.$$

Proof. As the matrix $\mathbf{G}_\ell$ is symmetric, we may find an orthogonal matrix $\mathbf{S}$ which diagonalizes it, i.e., with the property that ${}^t\mathbf{S}\mathbf{G}_\ell\mathbf{S} = \mathbf{D}$ is a diagonal matrix, whose diagonal entries are then, of course, the eigenvalues of $\mathbf{G}_\ell$ (taking into account multiplicities). We may thus assume

$$\mathbf{D} = \begin{pmatrix} n^\ell\mathbf{I}_{(n-1)\ell+1} & \mathbf{0} \\ \mathbf{0} & \mathbf{0} \end{pmatrix}.$$

Put $\mathbf{g} = \mathbf{S}\mathbf{f}$. Then, obviously, $\gamma_\ell(f) = n^\ell \sum_{i=0}^{(n-1)\ell} g_i^2$. The columns of the matrix $\mathbf{S}$ consist of (normalized) eigenvectors of $\mathbf{G}_\ell$. In particular, its first $(n-1)\ell+1$ columns may be chosen to be the normalizations of the vectors $\mathbf{v}_0^\ell, \ldots, \mathbf{v}_{(n-1)\ell}^\ell$ constructed before. So, let us consider the orthonormal basis

$$\{\mathbf{w}_0^\ell, \ldots, \mathbf{w}_{(n-1)(\ell-1)}^\ell, \mathbf{z}_1^\ell, \ldots, \mathbf{z}_{n-1}^\ell\}$$

of V_1^ℓ, where $\mathbf{w}_k^\ell = n^{-\ell/2}\mathbf{v}_k^\ell$ for $0 \leq k \leq (n-1)(\ell-1)$ and where $\mathbf{z}_i^\ell = (i^2 + i)^{-1/2}n^{(1-\ell)/2}\mathbf{v}_{(n-1)(\ell-1)+i}^\ell$ for $1 \leq i \leq n-1$.

We then obtain :

$$\begin{aligned}
\gamma_\ell(f) &= \gamma_\ell(f_0, \ldots, f_{n^\ell-1}) \\
&= n^\ell \sum_{k=0}^{(n-1)(\ell-1)} ({}^t\mathbf{w}_k^\ell\mathbf{f})^2 + n^\ell\sum_{i=1}^{n-1}({}^t\mathbf{z}_i^\ell\mathbf{f})^2 \\
&= n^\ell(n^{-\ell/2})^2 \sum_{k=0}^{(n-1)(\ell-1)} ({}^t\mathbf{v}_k^\ell\mathbf{f})^2 + n^\ell(n^{(1-\ell)/2})^2\sum_{i=1}^{n-1}\frac{1}{i(i+1)}({}^t\mathbf{v}_{(n-1)(\ell-1)+i}^\ell\mathbf{f})^2.
\end{aligned}$$

By construction, we thus obtain that $\gamma_\ell(f_0, \ldots, f_{n^\ell-1})$ is equal to

$$\begin{aligned}
&\gamma_{\ell-1}(f_0 + f_{n^{\ell-1}} + \ldots + f_{(n-1)n^{\ell-1}}, \ldots, f_{n^{\ell-1}-1} + \ldots + f_{n^\ell-1}) \\
&+n(\tfrac{1}{2}((f_0 + \ldots f_{n^{\ell-1}}) - (f_{n^{\ell-1}} + \ldots f_{2n^{\ell-1}-1}))^2 \\
&+\tfrac{1}{2.3}((f_0 + \ldots + f_{n^{\ell-1}-1}) + (f_{n^{\ell-1}} + \ldots + f_{2n^{\ell-1}-1}) - 2(f_{2n^{\ell-1}} + \ldots + f_{3n^{\ell-1}-1}))^2 \\
&+\ldots \\
&+\tfrac{1}{n(n-1)}((f_0 + \ldots + f_{n^{\ell-1}-1}) + \ldots - (n-1)(f_{(n-1)n^{\ell-1}} + \ldots + f_{n^\ell-1}))^2).
\end{aligned}$$

Let us write

$$\hat{\mathbf{f}} = \begin{pmatrix} f_0 + f_{n^{\ell-1}} + \ldots + f_{(n-1)n^{\ell-1}} \\ \vdots \\ f_{n^{\ell-1}-1} + \ldots + f_{n^\ell-1} \end{pmatrix} \in \mathbb{R}^{n^{\ell-1}}.$$

Then

$$\begin{aligned} ||\hat{\mathbf{f}}||^2 &= (f_0 + \ldots + f_{(n-1)n^{\ell-1}})^2 + \ldots + (f_{n^{\ell-1}-1} + \ldots + f_{n^\ell-1})^2 \\ &= f_0^2 + \ldots + f_{n^\ell-1}^2 + 2(f_0 f_{n^{\ell-1}} + \ldots + f_{n^{\ell-1}-1} f_{n^\ell-1}) = a^2, \end{aligned}$$

for some $a \geq 1$.

Let $\mathbf{f}' = \frac{1}{a}\hat{\mathbf{f}}$, then $||\mathbf{f}'|| = 1$ and

$$\gamma_{\ell-1}(f') = \gamma_{\ell-1}(\frac{1}{a}\hat{f}) = \frac{1}{a^2}\gamma_{\ell-1}(\hat{f}).$$

Let us now assume that for some positive integer ℓ, we have $\gamma_\ell(f) < n$, for some fitness function f with $||\mathbf{f}|| = 1$. Then

$$\begin{aligned} \gamma_{\ell-1}(\hat{f}) &\leq \gamma_{\ell-1}(\hat{f}) + \sum_{i=1}^{n-1} \frac{n}{i(i+1)}((f_0 + \ldots + f_{n^{\ell-1}-1}) + \ldots \\ &\quad -(i-1)(f_{(i-1)n^{\ell-1}} + \ldots + f_{in^{\ell-1}-1}))^2 \\ &= \gamma_\ell(f) < n. \end{aligned}$$

It follows that we thus also have

$$\gamma_{\ell-1}(f') = \frac{1}{a^2}\gamma_{\ell-1}(\hat{f}) < \frac{n}{a^2} \leq n.$$

Iterating this process, we would thus find some fitness function f with $||\mathbf{f}|| = 1$, and $\gamma_1(f) < n$. However, this is impossible, as γ_1 is easily seen to have constant value n on normalized fitness functions. This contradiction proves our assertion. ∎

5 Maximal epistasis revisited

We have already pointed out in the previous section that the minimal value $\gamma_\ell(f) = n$, corresponding to maximal normalized epistasis, may actually be reached. The main purpose of the present section is to solve the problem of completely describing the class of all fitness functions f for which $\gamma_\ell(f) = n$.

5.1. *Fix a positive integer $\ell \geq 2$ and consider mutually distinct indices $0 \leq i_0, \ldots, i_{n-1} \leq n^{\ell-1} - 1$, with the property that*

1. $\sum_{r=0}^{n-1} i_r = \frac{n}{2}(n^{\ell-1} - 1)$;

2. $d(i_r, i_s) = \ell - 1$ *for any* $0 \leq r \neq s \leq n - 1$.

For each such family of indices $i_0, \ldots, i_{n-1}$, we define

$$\mathbf{q}^{\ell}_{i_0 \ldots i_{n-1}} = \frac{\sqrt{n}}{n} \begin{pmatrix} \mathbf{e}_{i_0} \\ \vdots \\ \mathbf{e}_{i_{n-1}} \end{pmatrix} \in \mathbb{R}^{n^{\ell}},$$

where $\{\mathbf{e}_0, \ldots, \mathbf{e}_{n^{\ell-1}-1}\}$ is the canonical basis of $\mathbb{R}^{n^{\ell-1}}$.

For example, if $n = \ell = 2$, then we necessarily have $\{i_0, i_1\} = \{0, 1\}$ as suitable indices, and this corresponds to

$$\mathbf{q}^2_{0,1} = \frac{\sqrt{2}}{2} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \mathbf{q}^2_{1,0} = \frac{\sqrt{2}}{2} \begin{pmatrix} 0 \\ 1 \\ 1 \\ 0 \end{pmatrix}.$$

In general, still with $n = 2$, suitable indices are given by couples $0 \leq i_0, i_1 \leq 2^{\ell-1} - 1$, with $i_0 + i_1 = 2^{\ell-1} - 1$ (which automatically implies that $d(i_0, i_1) = \ell - 1$), and this yields vectors of the form

$$\mathbf{q}^{\ell}_{k, 2^{\ell-1}-k} = \frac{\sqrt{2}}{2} \begin{pmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} \in \mathbb{R}^{2^{\ell}}$$

with entry $\frac{\sqrt{2}}{2}$ at positions k and $2^{\ell} - k - 1$.

As another example, with $n = 3$ and $\ell = 2$, we necessarily have $\{i_0, i_1, i_2\} = \{0, 1, 2\}$ with, e.g.,

$$\mathbf{q}^2_{012} = \frac{\sqrt{3}}{3} \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \mathbf{q}^2_{102} = \frac{\sqrt{3}}{3} \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \\ 0 \\ 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}.$$

One should view the corresponding fitness functions $q^{\ell}_{i_0 \ldots i_{n-1}}$ as having n "peaks", lying as far apart as possible. Note also that suitable sets of indices $i_0, \ldots, i_{n-1}$ may *always be found. For example, putting*

$$i_r = r\frac{n^{\ell-1}-1}{n-1}$$

(with $0 \leq r \leq n-1$) obviously does the trick.

Let us now prove the following result, which completely answers the question mentioned at the beginning of this section :

Theorem. 5.2. *For any $\ell \geq 2$ and any positive $\mathbf{f} \in \mathbb{R}^{n^\ell}$ with $||\mathbf{f}|| = 1$, the following assertions are equivalent :*

1. $\varepsilon^*(f) = 1 - \frac{1}{n^{\ell-1}}$;
2. $\mathbf{f} = \mathbf{q}^{\ell}_{i_0 \ldots i_{n-1}}$ *for suitable indices* $0 \leq i_0, \ldots, i_{n-1} \leq n^{\ell-1} - 1$.

Proof. Let us start by proving that the second assertion implies the first one. For any choice of suitable indices $i_0, \ldots, i_{n-1}$ we have

$$\begin{aligned}
\gamma_\ell(f) &= {}^t\mathbf{f}\mathbf{G}_\ell\mathbf{f} = (\frac{\sqrt{n}}{n})^2({}^t\mathbf{e}_{i_0} \ldots {}^t\mathbf{e}_{i_{n-1}})\mathbf{G}_\ell \begin{pmatrix} \mathbf{e}_{i_0} \\ \vdots \\ \mathbf{e}_{i_{n-1}} \end{pmatrix} \\
&= \frac{1}{n}({}^t\mathbf{e}_{i_0} \ldots {}^t\mathbf{e}_{i_{n-1}}) \begin{pmatrix} g_{0,i_0} + g_{0,n^{\ell-1}+i_1} + \ldots + g_{0,(n-1)n^{\ell-1}+i_{n-1}} \\ \vdots \\ g_{n^\ell-1,i_0} + \ldots + g_{n^\ell-1,(n-1)n^{\ell-1}+i_{n-1}} \end{pmatrix} \\
&= \frac{1}{n}\{(g_{i_0,i_0} + \ldots + g_{i_0,(n-1)n^{\ell-1}+i_{n-1}}) + \ldots \\
&\quad \ldots + (g_{(n-1)n^{\ell-1}+i_{n-1},i_0} + \ldots + g_{(n-1)n^{\ell-1}+i_{n-1},(n-1)n^{\ell-1}+i_{n-1}})\} \\
&= \frac{1}{n}\{ng_{00} + 2((g_{i_0,n^{\ell-1}+i_1} + \ldots + g_{i_0,(n-1)n^{\ell-1}+i_{n-1}}) + \ldots \\
&\quad \ldots + (g_{(n-2)n^{\ell-1}+i_{n-2},(n-1)n^{\ell-1}+i_{n-1}}))\} \\
&= \frac{1}{n}\{n((n-1)\ell+1) + 2\{(n-1)((n-1)\ell+1) \\
&\quad -n(d_{i_0,n^{\ell-1}+1} + \ldots + d_{i_0,(n-1)n^{\ell-1}+i_{n-1}}) + (n-2)((n-1)\ell+1) \\
&\quad -n(d_{n^{\ell-1}+i_1,2n^{\ell-1}+i_2} + \ldots + d_{n^{\ell-1}+i_1,(n-1)n^{\ell-1}+i_{n-1}}) + \ldots \\
&\quad + \ldots + 1((n-1)\ell+1) - nd_{(n-2)n^{\ell-1}+i_{n-2},(n-1)n^{\ell-1}+i_{n-1}}\}\} \\
&= \frac{1}{n}\{((n-1)\ell+1)n^2 - 2n(d_{i_0,n^{\ell-1}+1} + \ldots + d_{(n-2)n^{\ell-1}+i_{n-2},(n-1)n^{\ell-1}+i_{n-1}})\} \\
&= n((n-1)\ell+1) - 2\begin{pmatrix} n \\ 2 \end{pmatrix}\ell = n,
\end{aligned}$$

which proves our claim.

To prove the converse, we will use induction on ℓ. Consider a fitness function f whose corresponding vector $\mathbf{f} \in \mathbb{R}^{n^\ell}$ is normalized and has the property that $\gamma_\ell(f) = n$. With notations as before, this means that

$$\begin{aligned}
n &= \gamma_\ell(f_0, \ldots, f_{n^\ell-1}) \\
&= \gamma_{\ell-1}(\hat{f}) + n\{\frac{1}{2}((f_0 + \ldots + f_{n^{\ell-1}-1}) - (f_{n^{\ell-1}} + \ldots + f_{2n^{\ell-1}-1}))^2 + \ldots \\
&\quad + \frac{1}{n(n-1)}((f_0 + \ldots + f_{n^{\ell-1}-1}) + \ldots - (n-1)(f_{(n-1)n^{\ell-1}} + \ldots + f_{n^\ell-1}))^2\},
\end{aligned}$$

hence

$$\gamma_{\ell-1}(\hat{f}) \leq \gamma_\ell(f).$$

Moreover,

$$\gamma_{\ell-1}(f') = \frac{1}{||\hat{\mathbf{f}}||^2}\gamma_{\ell-1}(\hat{f}) \leq \frac{1}{||\hat{\mathbf{f}}||^2}\gamma_\ell(f) \leq \frac{n}{||\hat{\mathbf{f}}||^2} \leq n,$$

so we necessarily have $\gamma_{\ell-1}(f') = n$, in view of the obtained lower bound on the value of γ_ℓ, and, of course, this yields $||\hat{\mathbf{f}}|| = 1$. We thus obtain $\hat{\mathbf{f}} = \mathbf{f}'$ and $\gamma_{\ell-1}(\hat{f}) = n$, whence the following identities :

$$\begin{aligned} f_0 + \ldots + f_{n^{\ell-1}-1} &= f_{n^{\ell-1}} + \ldots + f_{2n^{\ell-1}-1} \\ &= \ldots \\ &= f_{(n-1)n^{\ell-1}} + \ldots + f_{n^\ell-1}. \end{aligned}$$

On the other hand, as $||\hat{\mathbf{f}}|| = ||\mathbf{f}|| = 1$, we also have :

$$\begin{array}{ccccccccc} f_0 f_{n^{\ell-1}} & = & \ldots & = & f_0 f_{(n-1)n^{\ell-1}} & = & \ldots & = & f_{(n-2)n^{\ell-1}} f_{(n-1)n^{\ell-1}} & = & 0 \\ \vdots & & & & & & & & & & \\ f_i f_{n^{\ell-1}+i} & = & \ldots & = & f_i f_{(n-1)n^{\ell-1}+i} & = & \ldots & = & f_{(n-2)n^{\ell-1}+i} f_{(n-1)n^{\ell-1}+i} & = & 0 \\ \vdots & & & & & & & & & & \\ f_{n^{\ell-1}-1} f_{2n^{\ell-1}-1} & = & \ldots & = & f_{n^{\ell-1}-1} f_{n^\ell-1} & = & \ldots & = & f_{(n-1)n^{\ell-1}-1} f_{n^\ell-1} & = & 0 \end{array}$$

In particular, if $\ell = 2$ and $\gamma_2(f_0, \ldots, f_{n^2-1}) = n = \gamma_1(\hat{f})$, then the previous equations reduce to :

$$\begin{aligned} f_0 + \ldots + f_{n-1} &= f_n + \ldots + f_{2n-1} \\ &= \ldots \\ &= f_{(n-1)n} + \ldots + f_{n^2-1} \end{aligned}$$

and

$$\begin{array}{ccccccc} f_0 f_n & = & \ldots & = & f_{(n-2)n} f_{(n-1)n} & = & 0 \\ \vdots & & & & & & \\ f_{n-1} f_{2n-1} & = & \ldots & = & f_{(n-1)n-1} f_{n^2-1} & = & 0 \end{array}$$

Solving this system of equations easily yields that

$$\mathbf{f} = \frac{\sqrt{n}}{n} \begin{pmatrix} \mathbf{e}_{\sigma(0)} \\ \vdots \\ \mathbf{e}_{\sigma(n-1)} \end{pmatrix} = \mathbf{q}^2_{\sigma(0)\ldots\sigma(n-1)} \in \mathbb{R}^{n^2},$$

where σ is a permutation of $\{0, \ldots, n-1\}$ and $\{\mathbf{e}_0, \ldots, \mathbf{e}_{n-1}\}$ is the canonical basis of $\mathbb{R}^n$. Of course, if $0 \leq r \neq s \leq n-1$, then $\sigma(r) \neq \sigma(s)$ and

$$\sum_{r=0}^{n-1} \sigma(r) = \sum_{r=0}^{n-1} r = \frac{n}{2}(n-1),$$

so the indices $\sigma(0), \ldots, \sigma(r-1)$ satisfy the necessary requirements.

Let us now assume our assertion to hold true for strings of length $2, 3, \ldots, \ell - 1$ and let us prove it for length ℓ. Consider a normalized fitness function over strings of length ℓ and suppose that $\gamma_\ell(f) = n$. Then, by induction,

$$\hat{\mathbf{f}} = \mathbf{f}' = \mathbf{q}^{\ell-1}_{i_0\ldots i_{n-1}} \in \mathbb{R}^{n^{\ell-1}},$$

for indices $0 \le i_0, \ldots, i_{n-1} \le n^{\ell-2}-1$, with the property that $d(i_r, i_s) = \ell-1$ for $r \ne s$ and that $\sum_{r=0}^{n-1} i_r = \frac{n}{2}(n^{\ell-2} - 1)$. ¿From the very definition of $\hat{\mathbf{f}} = \mathbf{q}^{\ell-1}_{i_0\ldots i_{n-1}}$, it follows that its non-zero components may be found in the rows $kn^{\ell-2} + i_k$ $(0 \le k \le n-1)$, whose expression, for any k, is :

$$f_{kn^{\ell-2}+i_k} + f_{n^{\ell-1}+(kn^{\ell-2}+i_k)} + \ldots + f_{(n-1)n^{\ell-1}+(kn^{\ell-2}+i_k)} = \frac{\sqrt{n}}{n}.$$

On the other hand, the above systems of equations applied to $\hat{\mathbf{f}} = \mathbf{q}^{\ell-1}_{i_0\ldots i_{n-1}}$ reduce to :

$$\begin{aligned} & f_{i_0} + f_{n^{\ell-2}+i_1} + \ldots + f_{(n-1)n^{\ell-2}+i_{n-1}} = \ldots = \\ = \; & f_{(n-1)n^{\ell-1}+i_0} + f_{(n-1)n^{\ell-1}+(n^{\ell-2}+i_1)} + \ldots + f_{(n-1)n^{\ell-1}+((n-1)n^{\ell-2}+i_{n-1})} \end{aligned}$$

and

$$\begin{aligned} & f_{i_0} f_{n^{\ell-1}+i_0} = \ldots = \\ = \; & f_{i_0} f_{(n-1)n^{\ell-1}+i_0} = \ldots = \\ & \vdots \\ = \; & f_{(n-2)n^{\ell-1}+i_0} f_{(n-1)n^{\ell-1}+i_0} = 0 \\ & \vdots \\ & f_{(n-1)n^{\ell-2}+i_{n-1}} f_{n^{\ell-1}+((n-1)n^{\ell-2}+i_{n-1})} = \ldots = \\ = \; & f_{(n-1)n^{\ell-2}+i_{n-1}} f_{(n-1)n^{\ell-1}+((n-1)n^{\ell-2}+i_{n-1})} = \ldots = \\ = \; & f_{(n-2)n^{\ell-1}+((n-1)n^{\ell-2}+i_{n-1})} f_{(n-1)n^{\ell-1}+((n-1)n^{\ell-2}+i_{n-1})} = 0 \end{aligned}$$

Let us put $x^k_j = f_{jn^{\ell-1}+kn^{\ell-2}+i_k}$ for any $0 \le j, k \le n-1$, then the above systems of equations are equivalent to

$$(a)\left\{\begin{array}{lcl} x^0_0 + x^0_1 + \ldots + x^0_{n-1} & = & \frac{\sqrt{n}}{n} \\ & \vdots & \\ x^{n-1}_0 + \ldots + x^{n-1}_{n-1} & = & \frac{\sqrt{n}}{n} \end{array}\right.$$

$$(b)\left\{\begin{array}{l} x^0_0 + x^1_0 + \ldots + x^{n-1}_0 = \cdots = \\ x^0_{n-1} + x^1_{n-1} + \ldots + x^{n-1}_{n-1} \end{array}\right.$$

$$(c_1)\left\{\begin{array}{lclcl} x^0_0 x^1_0 & = & \ldots & = & x^0_0 x^{n-1}_0 \\ & & \ddots & & \\ & & & = & x^0_{n-2} x^0_{n-1} = 0 \end{array}\right.$$

$$\vdots$$

$$
(c_{n-1}) \begin{cases} x_0^{n-1}x_1^{n-1} &= \ldots = x_0^{n-1}x_{n-1}^{n-1} \\ & \ddots \\ & = x_{n-2}^{n-1}x_{n-1}^{n-1} = 0 \end{cases}
$$

In view of the fact that $x_j^k \geq 0$ for all indices j, k, it follows that in each of the equations in (a) at least one of the summands has to be non-zero. The equations (c) imply the unicity of this summand. It thus follows that the system of equations (a) reduces to

$$
x_{r_0}^0 = x_{r_1}^1 = \ldots = x_{r_{n-1}}^{n-1} = \frac{\sqrt{n}}{n}
$$

for certain $0 \leq r_i \leq n-1$. Moreover, analyzing the equations (b), it follows that in each of the composing equations there should be the same number of non-zero terms. A tedious, but essentially straightforward verification, shows that in each of them there is actually exactly just one non-zero component. The solutions are thus of the form

$$
x_{r_0}^0 = x_{r_1}^1 = \ldots = x_{r_{n-1}}^{n-1} = \frac{\sqrt{n}}{n}
$$

with $r_i \neq r_j$ if $i \neq j$. In other words,

$$
\mathbf{f} = \frac{\sqrt{n}}{n} \begin{pmatrix} \mathbf{e}_{\hat{\imath}_0} \\ \vdots \\ \mathbf{e}_{\hat{\imath}_{n-1}} \end{pmatrix} \in \mathbb{R}^{n^\ell}
$$

where $\hat{\imath}_j = pn^{\ell-2} + i_p$ for some suitable indices i_p, such that the $0 \leq \hat{\imath}_0, \ldots, \hat{\imath}_{n-1} \leq n^{\ell-1} - 1$ are mutually distinct, and such that

$$
\begin{aligned}
\textstyle\sum_{r=0}^{n-1} \hat{\imath}_r &= \textstyle\sum_{r=0}^{n-1} i_r + \sum_{r=0}^{n-1} rn^{\ell-2} \\
&= \tfrac{n}{2}(n^{\ell-2} - 1) + n^{\ell-2}(\tfrac{n(n-1)}{2}) \\
&= \tfrac{n}{2}(n^{\ell-1} - 1)
\end{aligned}
$$

and

$$
d(\hat{\imath}_j, \hat{\imath}_k) = d(pn^{\ell-2} + i_p, qn^{\ell-2} + i_q) = 1 + d(i_p, i_q) = 1 + (\ell - 1) = \ell.
$$

This finishes the proof. ∎

5.3. *Let us interpret this result in the binary case, for simplicity's sake. In this case, the maximal value for normalized epistasis is* $1 - \frac{1}{2^{\ell-1}}$ *and is reached by fitness functions* c*, which are zero everywhere, except for two points at maximal Hamming distance (e.g.,* $0 \ldots 0$ *and* $1 \ldots 1$*), with equal fitness value.*

Although both c *and the "Dirac function"* d *(with single peak at* $1 \ldots 1$*, e.g.) are both hard (optimalization essentially reduces to random search), at first glance, it might seem strange that* c *is more difficult to optimize by the GA than* d*. However, one should take into account the fact that the maximum* m *of* d *is more stable than the two maxima* m_1 *and* m_2 *of* c*, in the following sense.*

Once the maximum m *of* d *is discovered, the simple GA will continue selecting* m *with a high probability, due to its high fitness. Combined with a point different from* m*, crossover is, of course, highly probable to eliminate* m*. On the other hand,* *crossover will almost always use two copies of* m*, due to its high selection probability, and this will not only make* m *survive, but even produce more copies of* m *in the population.*

In the case of the fitness c*, things are different, since both* m_1 *and* m_2 *have (equal) high probability of being selected. If only* m_1 *is encountered in the initial population or through random search and if* m_2 *remains undiscovered for a "long enough period",* m_1 *will also tend to dominate, just as in the previous case. However, if* m_2 *is also present, in equal proportion as* m_1*, copies of* m_1 *and* m_2 *have equal (high) probability of being selected. Crossover between* m_1 *and* m_2 *destroys both of them however, leading the GA away from these maxima.*

Of course, in practical situations, i.e., with large lengths ℓ*, both functions have the same normalized epistasis (approximately equal to 1.00), the previous result thus mainly being of theoretical interest. Moreover, the above phenomenon only will occur within large populations, forcing both maxima* m_1 *and* m_2 *to occur with equal frequency.*

We experimentally verified the behaviour just described, using $G(f)$ *as an indicator for GA-hardness, as in 1.4. We worked with strings of length 4, with a (large) population of size 200. We then found :*

f	$G(f)$	ε^*_ℓ
R^2_0	7	0.00
R^2_1	8	0.20
R^2_2	13	0.69
c	20	0.87

(Note that R^2_2 *is just the "Dirac" function, centered at 1111).*

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M. T. Iglesias – C. Vidal
Universidad de La Coruña
Facultad de Informática
La Coruña, España

D. Suys – A. Verschoren
University of Antwerp, RUCA
Department of Mathematics and Computer Science
Antwerpen, Belgium