Computing epistasis of Generalized Royal Road functions using Walsh transforms and the Hyperplane averaging theorem

M.T. Iglesias[†**], Vicente S. Peñaranda[†] and A. Verschoren[*]

[†] Universidade da Coruña, Spain. (totero@udc.es, vesp@udc.es)
[*] Universiteit Antwerpen, Belgium. (alain.verschoren@ua.ac.be)
[**] Research partially supported by a grant of Xunta de Galicia, PGIDIT03PXIA10502PR

Abstract

Genetic Algorithms (*GA*) are a mathematical tool based on the mechanisms of the evolution of species and are successfully applied mainly as function optimizers. They look for the most fit solution for a particular problem, by means of the evolution of populations of data that, once codified –generally a binary encoding– use *genetic operators* which iteratively produce new and better individuals (binary vectors), in an *adaptive search process* that eventually tends to converge to an optimum.

Many search techniques need much auxiliary information in order to work properly (gradient techniques require derivatives, for instance). By contrast, GA have no need for all this auxiliary information. As Goldberg says in [2]: "GAs are blind. To perform an effective search for better and better structures, they only require payoff values (objetive function values) associated with individual strings". For that reason, they are an adequate tool for search and optimization where the classical methods are not viable.

If a GA cannot find the optimum of a function in a reasonable amount of time, then this function is said to be *GA-hard*. The characterization of these "difficult" functions still remains open. In 1991 Davidor tackled this phenomenon by noting that in Genetics the interaction between the genes affects the characteristics of an individual (*epistasis*[1]) and transferred this approach to the present context, where the epistasis measures how the suitability of a candidate optimum depends on the interaction between the different components of the vector representing it. The mathematical formalization of this concept heavily depends on basic linear algebra and allows to numerically estimate the difficulty of a large class of problems. More concretely, associate to any real valued function f the vector

$$^t\mathbf{f} = \big(f(00\ldots0),\quad f(00\ldots1),\quad \cdots,\quad f(11\ldots1)\big) = \big(\mathrm{f}_0,\quad \mathrm{f}_1,\quad \cdots,\quad \mathrm{f}_{2^\ell-1}\big),$$

and consider the 2^ℓ-dimensional matrix $\mathbf{E}_\ell = (e_{ij}) \in M_{2^\ell}(\mathbb{R})$ $(0 \leq i,j \leq 2^\ell - 1)$, with $e_{ij} = 2^{-\ell}(\ell + 1 - 2\mathrm{d}_{ij})$, where d_{ij} denotes the Hamming distance between i and j. In 1995, Van Hove uses the generalized inverse of the matrix $\mathbf{E}_\ell$ to calculate the distance between any fitness function and its projection on a space of linear functions, as a means to describe its epistasis. In 1996, Suys and Verschoren note that $\mathbf{E}_\ell$ is an orthogonal projection and define the *normalized epistasis* of a fitness function f as $\varepsilon^*(f) = 1 - \frac{^t\mathbf{f}\,\mathbf{E}_\ell\mathbf{f}}{^t\mathbf{f}\,\mathbf{f}}$. In particular, $0 \leq \varepsilon^*(f) \leq 1$. Moreover, it appears that the functions with extreme epistasis value are rather easy to characterize as, for examples, the functions with $\varepsilon^*(f) = 0$ are, not unexpectedly, exactly the linear functions.

Although the presence of epistasis is by no means sufficient to completely predict GA-hardness, for large classes of functions (mainly those characterized by a small number of structural parameters), there is a strong link between experimental results leading to estimates of

[1]It derives from Greek words *epis* and *stasis* ("behind" and "stand".)

GA hardness and theoretical calculations involving normalized epistasis. As an example of this phenomenon, let us mention the so-called generalized Royal Road functions R^n_m defined over binary strings $s = s_{\ell-1} \dots s_0 \in \{0,1\}^{2^n}$ (of length 2^n) by $R^n_m(s) = \sum_{s \in \sigma_p^{n,m}} 2^m$ where, we denote by $\sigma_p^{n,m}$ the schemata $\#^{(2^m p)} 1^{(2^m)} \#^{2^n - 2^m(p+1)}$, $(0 \le p < 2^{n-m})$, i.e.,

$$\sigma_p^{n,m} = \{s \in \{0,1\}^{2^n};\ s_j \neq \# \Rightarrow s_j = 1\}.$$

Unfortunately, calculating the epistasis directly from its algebraic expression is, in general, very complicated. As an example, let us just point out the extremely long and tedious calculation for the functions R^n_m by Naudts, Suys and Verschoren, where the epistasis explains very well the strange behavior of these functions, which are GA-hard in spite of their easy structure.

In order to avoid the complex calculations just referred to, in this poster we show how the application of an appropriate change of basis allows us to write the functions R^n_m in terms of their so -called *Walsh coeficients*.

It is well known that the Walsh functions, which we denote by $\{\psi_t,\ t \in \Omega_\ell\}$, –where, for any $t \in \Omega_\ell$, ψ_t is given by $\psi_t(s) = (-1)^{s \cdot t}$ ($s \cdot t$ is the scalar product of s and t)–, form a basis for the vector space of real valued functions on $\Omega_\ell = \{0,1\}^\ell$. In fact, if we consider the 2^ℓ-dimensional matrix, $\mathbf{V}_\ell = (\psi_t(s))_{s,t}$, –which completely determines the Walsh functions– and if we represent any function f by its associated vector $\mathbf{f}$, then the components $\omega_i = \omega_i(f)$ of the *Walsh transform* ω of f –the so-called *Walsh coefficients* of f– are (up to a normalization factor) just the coordinates of f with respect to this basis. The Walsh transform of f is determined by its associated vector $\mathbf{w} = \mathbf{W}_\ell \mathbf{f}$, where the idempotent matrix $\mathbf{W}_\ell = 2^{-\ell/2}\mathbf{V}_\ell$ verifies the recursion relation:

$$\mathbf{W}_{\ell+1} = 2^{-\frac{1}{2}} \begin{pmatrix} \mathbf{W}_\ell & \mathbf{W}_\ell \\ \mathbf{W}_\ell & -\mathbf{W}_\ell \end{pmatrix}.$$

Moreover, as $\mathbf{W}_\ell \mathbf{E}_\ell \mathbf{W}_\ell = \mathbf{D}_\ell$, where $\mathbf{D}$ is the diagonal matrix whose only non-zero entries have value 1 and are situated at $i = 0$ and $i = 2^j$, $0 < j \le \ell - 1$, Naudts et al easily showed that

$$\varepsilon^*_\ell(f) = 1 - \frac{\omega_0^2 + \sum_{i=0}^{\ell-1} \omega_{2^i}^2}{\sum_{j=0}^{2^\ell - 1} \omega_j^2}. \qquad (1)$$

Using this expression, as well as the *Hyperplane Average Theorem*, which relates the suitability of a scheme to the Walsh coefficients of the fitness function, we were able to greatly simplify the calculations of the epistasis of the generalized Royal Road functions, by using the fact that to calculate the epistasis of R^n_m it suffices to calculate only a few Walsh coefficients. In particular, we obtain $\omega_0 = 2^{n-m}\ \omega$ with $\omega = 2^{m + 2^{n-1} - 2^m}$ and, for any $i_1, ..., i_k \in \{0, ..., 2^n - 1\}$,

$$\omega_{2^{i_1} + \dots + 2^{i_k}} = \begin{cases} (-1)^k \omega & \text{if } j \cdot 2^m \le i_1, ..., i_k < (j+1) \cdot 2^{m+1},\ 0 \le j < 2^n \\ 0 & \text{elsewhere.} \end{cases}$$

Now, from identity (1) we easily obtain $\varepsilon^*(R^n_m) = \frac{2^{2^m} - 2^m - 1}{2^{2^m} + 2^{n-m} - 1}$.

This method opens alternative means to calculate the *epistasis* of other functions.

References

[1] Y. Davidor, *Epistasis and Variance: A Viewpoint on GA-Hardness*, Foundations of Genetic Algorithms 1, 23-25. Ed. G.J.E. Rawlins, Morgan Kaufmann Publishers, San Mateo, 1991.

[2] D. E. Goldberg, Genetic Algorithms in Search, Optimization and Machine Learning, Addison Wesley Longman, Inc, 1989.

[3] D. E. Goldberg, *Genetic Algorithms and Walsh functions: Part I, A Gentle Introduction*, Complex Systems 3, 129-152, 1989.

[4] J. H. Holland, *Adaptation in Natural and Artificial Systems*, 5^a ed. Massachusetts Institute of Tecnology, MIT Press, 1998.

[5] B. Naudts, D. Suys and A. Verschoren, *Epistasis, Deceptivity and Walsh Transforms*, Proceedings of the International ICSC Symposium on Engineering of Intelligent Systems (EIS'98), vol 1: Fuzzy Logic/Genetic Algorithms, ICSC Academic Press, 210-216, 1998.

[6] B. Naudts, D. Suys and A. Verschoren, *Generalized Royal Road functions and their Epistasis*, Artificial Intelligence, vol 19, 317-334, 2000.

[7] G. Strang, *Linear Algebra and its Applications*, Academic Press, 1976.

[8] D. Suys and A. Verschoren, *Extreme Epistasis*, International Conference on Intelligent Technologies in Human-Relates Sciencies (ITHURS 96), vol II, 251-258, León, 1996.

[9] H. Van Hove, *Representational Issues in Genetic Algorithms*, Ph. D. Thesis. University of Antwerp, 1995.