Random Walks and Orthogonal Functions Associated with Highly Symmetric Graphs

By

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Abstract

The relationship of orthogonal functions associated with vertex transitive graphs and random walks on such graphs is investigated. We use this relations to characterize the exponentially decaying autocorrelation functions along random walks on isotropic random fields defined on vertex transitive graphs. The results are applied to a simple spin glass model.

Motivation

Recently "combinatory landscapes" — maps from the vertex set of some graph into the real or complex numbers — have received increasing attention. The classic example from physics is a Hamiltonian that assigns an energy value to a spin configuration (Mézard *et al.* 1987). Combinatorial optimization problems, like the travelling salesman problem (Lawler *et al.* 1985), are of the same type. In evolutionary biology maps assigning free energies or "fitness values" to biomolecules — encoded as strings over a finite alphabet — are of particular interest (Eigen *et al.* 1989, Fontana *et al.* 1991, 1992). For each of these models the set of all possible configurations can be viewed as the vertex set V of a finite connected graph Γ. The edges of Γ are defined by elementary transformations of the configurations, like flipping a single spin in a spin glass or exchanging the order of two cities in a tour of the TSP.

It has been proposed to characterize landscapes by means of the time series sampled along a random walk on Γ (Eigen *et al.* 1989, Weinberger 1990). To be precise, consider a random field $\mathcal{F}$ on Γ (Besag 1974) defined by the probabilities

$$P(y_1, y_2, \ldots, y_{|V|}) = \text{Prob}\left\{(t_1, t_2, \ldots, t_{|V|}) \,\middle|\, -\infty < t_i \le y_i \,\forall\, i \in V\right\} \qquad (1)$$

The m-th moments of this random field are given by

$$M_{i_1 i_2 \ldots i_m} = \int_{\mathbb{R}^{|V|}} y_{i_1} y_{i_2} \ldots y_{i_m} \, dP(y_1, y_2, \ldots, y_{|V|}) \qquad (2)$$

For applications the most interesting quantity is the covariance matrix

$$R_{pq} = M_{pq} - M_p M_q \tag{3}$$

A random field on Γ is *isotropic* if (i) $M_p = \mu$ for all $p \in V$ and (ii) if $R_{pq} = R_{st}$ whenever there is an automorphism α of the graph with $s = \alpha(p)$ and $t = \alpha(q)$. In biological applications Γ is usually distance transitive, i.e., for any two pairs of vertices p, q and r, t with $d(s,t) = d(p,q)$ there is an automorphism α of Γ with $r = \alpha(p)$ and $t = \alpha(q)$, where $d(\,.\,,\,.\,)$ denotes the canonical distance on Γ. Consequently, the autocorrelation function of an isotropic random field on a distance transitive graph is of the form

$$\rho(d) = R_{pq}/R_{pp} \qquad \forall\, p,q \qquad \text{such that} \quad d(p,q) = d \tag{4}$$

A *simple random walk* on a graph Γ is obtained by choosing each of the neighboring vertex with probability $1/\deg(x)$, where $\deg(x)$ denotes the vertex degree of x. Let A denote the adjacency matrix of Γ, which is defined by $a_{ij} = 1$ if $d(i,j) = 1$ and $a_{ij} = 0$ otherwise. The transition matrix of a simple random walk is therefore $t_{yx} = a_{yx}/\deg(x)$. Any such walk $\{x_0, x_1, \ldots\}$ induces a time series $\{y_0, y_1, \ldots\}$ on an instance of the random field $\mathcal{F}$. In this contribution we investigate the relationship of the autocorrelation functions $r(s)$ of this time series and the "landscape" autocorrelation function $\rho(d)$.

Orthogonal Functions of Highly Symmetric Graphs

Let Γ be a distance transitive graph with adjacency matrix A. Following Biggs (1974) we define

$$s_{ijk} = \Big|\ \big\{x \in V(\Gamma) \big|\, d(z,x) = i,\ d(x,y) = j\big\}\ \Big| \qquad k = d(y,z) \tag{5}$$

The *intersection numbers* are independent of the choice of the "reference vertex" $z \in V$. Without loosing generality we will denote the reference vertex by 0 in the following. Let $\mathcal{N}(k)$ denote the set of vertices $x \in V$ fulfilling $k = d(0,x)$, and let $N(k) = |\mathcal{N}(k)|$ be its size. Let D be the diameter of Γ. Then

$$b_{ik} := s_{i1k} = \sum_{x \in \mathcal{N}(i)} A_{xy} \qquad \text{for all } y \in \mathcal{N}(k), \quad 0 \le k \le D \tag{6}$$

This $(D+1) \times (D+1)$-matrix B is known as the *intersection matrix* of Γ.

More generally, let Γ be a vertex transitive graph, i.e., for each pair of vertices $x, y \in V$ there is an automorphism α fulfilling $x = \alpha(y)$. Let us consider a partition of the vertex set V into M subsets $\mathcal{V}(0) = \{0\}$, $\mathcal{V}(1)$, $\mathcal{V}(2)$, …, $\mathcal{V}(M)$ such that

$$c_{ij} := \sum_{x \in \mathcal{V}(i)} A_{xy} \qquad \text{independent of } y \in \mathcal{V}(j). \tag{7}$$

In the worst case each subset contains a single vertex. For highly symmetric graphs, however, the *collapsed adjacency matrix* $C = (c_{ij})$ can be much smaller than the adjacency matrix A (see e.g. Bollobás 1979). In case of distance transitive graphs, for instance, the distance classes $\mathcal{N}(i)$ form a partition fulfilling equ.(7), and the collapsed adjacency matrix C coincides with the intersection matrix B defined in equ.(5) (Biggs 1974, Cvetković *et al.* 1980).

In the following we will use the letters $x, y, \ldots$ for vertices of the graph and the letters i, j, k, l, p, q for labelling subsets of V. A component of a vector v is denoted by $v(i)$ as we need indices to distinguish vectors.

Lemma 1. *Let e be an eigenvector of A with eigenvalue λ. Then v defined by*

$$v(p) = \sum_{x \in \mathcal{V}(p)} e(x) \tag{8}$$

is a right eigenvector of C with the same eigenvalue. The components of a left eigenvector are given by

$$u(p) = \frac{1}{|\mathcal{V}(p)|} v(p). \tag{9}$$

Furhtermore we have $u(0) = v(0) = 1/\sqrt{|V|}$ for all normalized eigenvectors of C.

Proof. From equations (7) and (8) we find

$$\begin{aligned}\lambda v(i) &= \lambda \sum_{x\in\mathcal{V}(i)} e(x) = \sum_{x\in\mathcal{V}(i)} \sum_{y\in V} A_{xy} e(y) = \\ &= \sum_{k=0}^{M} \sum_{y\in\mathcal{V}(k)} \sum_{x\in\mathcal{V}(i)} A_{xy} e(y) = \sum_{k=0}^{M} \sum_{y\in\mathcal{V}(k)} e(y) c_{ik} = \\ &= \sum_{k=0}^{D} c_{ik} v(k) = (Cv)(i).\end{aligned}$$

Equ.(7) implies

$$c_{kl} = \frac{1}{|\mathcal{V}(l)|} \sum_{y\in\mathcal{V}(l)} \sum_{x\in\mathcal{V}(k)} A_{xy}, \qquad c_{lk} = \frac{1}{|\mathcal{V}(k)|} \sum_{x\in\mathcal{V}(k)} \sum_{y\in\mathcal{V}(l)} A_{yx} \tag{10}$$

and by symmetry of A we have

$$c_{kl} = |\mathcal{V}(k)|/|\mathcal{V}(l)|\, c_{lk}. \tag{11}$$

Hence $(uC)(k) = \sum_{j=0}^{M} u(j) c_{jk} = \frac{1}{|\mathcal{V}(k)|} \sum_{j=0}^{M} c_{kj} v(j) = \frac{1}{|\mathcal{V}(k)|} \lambda v(k) = \lambda u(k)$.

As an immediate consequence we have $u(0) = v(0) = e(0)$ for all eigenvectors of C. Since A is symmetric we may arrange the eigenvectors $e_z(x)$ in a unitary matrix, i.e., such that $e_z(x) = e_x^*(z)$. The theorem of Perron-Frobenius ensures that $\lambda_0 = N(1)$ (the vertex degree of Γ) is a simple eigenvalue with normalized eigenvector $e_0(x) = 1/\sqrt{|V|}$. Eqns.(7) and (8) shown $u(0) = e_x(0) = e_0(x) = 1/\sqrt{|V|}$. ∎

Remark. If λ is a simple eigenvalue of C then equ.(8) holds for all vectors e in the eigenspace of A belonging to λ. Biggs (1974) proved for distance transitive graphs that A and B have the same spectrum, and that B has $D+1$ simple eigenvalues. For distance transitive graphs, the *left* eigenvectors u_d, $d = 0, 1, \ldots D$, of B are known as orthogonal (or spherical) functions associated with the graph Γ (Dunkl 1979).

Simple Random Walks on Vertex Transitive Graphs

A simple random walk on Γ starting at vertex 0 is a Markov process with transition matrix

$$T = \frac{1}{N(1)} A \tag{12}$$

and initial condition $\pi_0(x) = \delta_{0x}$. (Here δ_{ij} is Kronecker's symbol defined by $\delta_{ii} = 1$ and $\delta_{ij} = 0$ for $i \neq j$.) Since Γ is connected, T is an irreducible bistochastic matrix. The probabilities $\varphi_{s\kappa}$ that a random walk starting at 0 reaches a vertex in partition $\mathcal{V}(\kappa)$ can be used to describe the relaxation of the random walk. They are immediately obtained from the transition matrix of the underlying Markov process:

$$\varphi_{s\kappa} := \sum_{x \in \mathcal{V}(\kappa)} \sum_{y \in V} [T^s]_{xy} \pi_0(y) \tag{13}$$

Lemma 2.

$$\varphi_{s\kappa} = \frac{1}{\sqrt{|V|}} \sum_{p=0}^{M} g_p \lambda_p^s \tilde{v}_p(\kappa) \tag{14}$$

where λ_p is eigenvalue of T, $\{\tilde{v}_p\}$ is an orthogonal basis of right eigenvectors of C normalized such that $\tilde{v}_p(0) = 1/\sqrt{|V|}$ and $g_p > 0$.

Proof. We expand π_0 in terms of the eigenvectors e_z,

$$\pi_0(y) = \frac{1}{\sqrt{|V|}} \sum_{z \in V} e_z(y), \tag{15}$$

and substitute this into equation (13):

$$
\begin{aligned}
\varphi_{s\kappa} &= \frac{1}{\sqrt{|V|}} \sum_{x\in\mathcal{V}(\kappa)} \sum_{y\in V} [T^s]_{xy} \sum_{z\in V} e_z(y) = \\
&= \frac{1}{\sqrt{|V|}} \sum_{z\in V} \sum_{x\in\mathcal{V}(\kappa)} \sum_{y\in V} [T^s]_{xy} e_z(y) = \\
&= \frac{1}{\sqrt{|V|}} \sum_{z\in V} \sum_{x\in\mathcal{V}(\kappa)} \lambda_z^s e_z(x) = \\
&= \frac{1}{\sqrt{|V|}} \sum_{z\in V} \lambda_z^s v_z(\kappa).
\end{aligned} \tag{16}
$$

Here λ_z denotes the eigenvalue of T with eigenvector e_z, v_z is the corresponding eigenvector of C, as defined by equ.(8).

Let E_r be the (right) eigenspace corresponding to eigenvalue λ_r, and let $\{\tilde{v}_1, \ldots, \tilde{v}_h\}$, $h = \dim E_r$, be a basis of E_r which is orthogonal with respect to the scalar product

$$
\langle a; b\rangle \;=\; \sum_{p=0}^{M} \frac{a(p)b(p)}{|\mathcal{V}(p)|} \tag{17}
$$

Then $\{\tilde{u}_1, \ldots, \tilde{u}_h\}$, defined by $\tilde{v}_i(p) = |\mathcal{V}(p)|\tilde{u}_i(p)$, is a basis of the corresponding left eigenspace. By construction we have

$$
\sum_{p=0}^{M} \tilde{u}_i(p)\tilde{v}_j(p) = \langle \tilde{v}_i; \tilde{v}_j\rangle = N_i\delta_{ij} \tag{18}
$$

with $N_i > 0$. Furthermore the basis vectors $\tilde{u}_i$ can be chosen such that

$$
\tilde{u}_i(0) = \tilde{v}_i(0) = 1/\sqrt{|V|} \tag{19}
$$

since at least one eigenvector of each eigenvalue is of this form as a consequence of lemma 1. Thus equ.(16) may be written in the form of equ.(14) with some coefficients g_p. That $g_p > 0$ will be proved together with the main result of this paper in the next section. ∎

Remark. If all eigenvalues of C are simple then equ.(14) simplifies to

$$\varphi_{s\kappa} = \frac{1}{\sqrt{|V|}} \sum_{p=0}^{M} m(\lambda_p)\lambda_p^s v_p(\kappa) \tag{20}$$

where $m(\lambda)$ denotes the multiplicity of an eigenvalue λ of A.

Main Theorem

Consider a function $\hat{\rho} : V \times V \longrightarrow \mathbb{C}$ such that $\hat{\rho}(x, y) = \rho(\kappa)$ whenever there is an automorphism of Γ such that $\alpha(x) = 0$ and $\alpha(y) \in \mathcal{V}(\kappa)$. For any such function we define

$$r : \mathbb{N}_0 \longrightarrow \mathbb{C}\,, \qquad r(s) = \sum_{\kappa=0}^{M} \varphi_{s\kappa}\rho(\kappa) \tag{21}$$

A simple random walk $\{x_0, x_1, \ldots\}$ on Γ generates a time series $\{\hat{\rho}(x_0, x_0)$, $\hat{\rho}(x_0, x_1)$, $\ldots\}$. Then $r(s)$ is the expectation of the s-th point of this series. Obviously we have $r(0) = \rho(0) = \hat{\rho}(x_0, x_0)$ for all $x_0 \in V$. If we choose $\hat{\rho}(p, q) = R_{pq}$, the covariance matrix of an isotropic random field, then $r(s)$ is the autocorrelation function along the random walk.

Theorem. *The the function r along a random walk is a decaying exponential if and only if ρ is a left eigenvector with positive eigenvalue of the collapsed adjacency matric C.*

Proof. $\rho(\kappa)$ may be expanded in terms of the *left* eigenvectors of C,

$$\rho(\kappa) = \sum_{l=0}^{M} a_l \tilde{u}_l(\kappa). \tag{22}$$

Inserting into equation (15) yields

$$\begin{aligned} r(s) &= \frac{1}{\sqrt{|V|}} \sum_{d=0}^{M}\sum_{l=0}^{M}\sum_{p=0}^{M} a_l \tilde{u}_l(d)\lambda_p^s \tilde{v}_p(d) g_p = \\ &= \frac{1}{\sqrt{|V|}} \sum_{p=0}^{M} \lambda_p^s g_p \sum_{l=0}^{M} a_l \sum_{d=0}^{M} \tilde{u}_l(d)\tilde{v}_p(d) = \\ &= \frac{1}{\sqrt{|V|}} \sum_{p=0}^{M}\sum_{l=0}^{M} a_l g_p N_l \delta_{pl} \lambda_p^s = \\ &= \frac{1}{\sqrt{|V|}} \sum_{l=0}^{M} a_l g_l N_l \lambda_l^s \end{aligned} \tag{23}$$

Choosing $a_l = \sqrt{|V|}\delta_{lf}$ we find $1 = \rho(0) = r(0) = g_f N_f = 1$. (This proves the missing part of lemma 2, since $g_f = 1/N_f > 0$). Equ.(23) finally simplifies to

$$r(s) = \frac{1}{\sqrt{|V|}} \sum_{l=0}^{M} a_l \lambda_l^s. \tag{24}$$

Therefore $r(s)$ is a decaying exponential if and only if all non-zero coefficients a_l belong to the same (positive) eigenvalue, say λ_r, i.e., if and only if $\rho \in E_r$ and $\lambda_r > 0$. ∎

Corollary. Equ.(14) is equivalent to

$$\varphi_{s\kappa} = \frac{1}{\sqrt{|V|}} \sum_{p=0}^{M} \frac{\tilde{v}_p(\kappa)}{\langle \tilde{v}_p; v_p \rangle} \lambda_p^s \tag{25}$$

If all eigenvalues of C are simple then $\langle \tilde{v}_p; v_p \rangle = m(\lambda_p)$

Corollary. If Γ is not bipartite then

$$\lim_{s\to\infty} r(s) = 0 \qquad \Longleftrightarrow \qquad \sum_{\kappa=0}^{M} |\mathcal{V}(\kappa)| \rho(\kappa) = 0. \tag{26}$$

If Γ is bipartite then only ($\Longrightarrow$) holds. For the converse we need additionally that $\lim_{s\to\infty} r(s)$ exists.

Corrolary. The random walk autocorrelation function $r(s)$ of an isotropic random field is a superposition of at most L exponential functions, where L is the number of distinct eigenvalues of the underlying graph.

Corollary. Let Γ be distance transitive and $r(s) = \tau^s$ for some $0 < \tau < 1$. Then (i) τ is an eigenvalue of T belonging to, say, distance class q, and (ii) the landscape autocorrelation function is of the form

$$\rho(d) = \sqrt{|V|}\, u_q(d). \tag{27}$$

Corrolary. Consider an isotropic random field $\mathcal{F}$ on a vertex transitive graph Γ. The time series along a simple random walk is uncorrelated, $r(s) =$

δ_{0s}, if and only if the autocorrelation function $\rho(\kappa)$ of $\mathcal{F}$ is eigenvector of C with eigenvalue 0. Note that a graph need not have an eigenvalue 0, and hence there are graphs for which no random field exists that gives rise to an uncorrelated time series of a simple random walk. Simple examples are the Boolean Hypercube graph with odd diameter.

Corrollary. Let $\mathcal{F}$ be an uncorrelated random field on Γ, i.e., $\rho(\kappa) = \delta_{0\kappa}$. Then

$$r(s) = \frac{1}{|V|}\mathrm{Tr}\ T^s = \frac{1}{|V|}\sum_k m(\lambda_k)\lambda_k^s \tag{28}$$

and, in particular, $r(1) = 0$, $r(2) = 1/N(1)$, and $r(2n) > 0$ for all $n \in \mathbb{N}$.

Application: Long Range Spin Glasses

The p-spin model has the Hamiltonian

$$\mathcal{H}_p(x) = \sum_{i_1<i_2<\dots i_p} J_{i_1 i_2 \dots i_p}\, x_{i_1} x_{i_2} \dots x_{i_p} \tag{29}$$

with $x_k = \pm 1$, $1 \le k \le n$. The coupling constants $J_{i_1 i_2 \dots i_p}$ are uncorrelated and independently distributed random variables drawn from a common distribution with finite variance and mean 0. The set of all configurations $x = (x_{i_1} x_{i_2} \dots x_{i_p})$ forms a distance transitive graph known as Boolean Hypercube by identifying x with a vertex and connecting two vertices x and y if they differ in a single position, i.e., if there is exactly one j with $x_j = -y_j$. The distance on Γ coincides with the Hamming distance, i.e., with the number of positions in which two configurations differ. The special case $p = 2$ is known as Sherrington-Kirkpatrick spin glass (Sherrington and Kirkpatrick 1975).

The covariance matrix of this model can be obtained exactly from

$$R_{xy} = \mathcal{E}[\mathcal{H}_p(x)\mathcal{H}_p(y)] = \sum_{i_1<i_2<\dots i_p} \mathcal{E}[J^2_{i_1 i_2 \dots i_p}] x_{i_1} y_{i_1} \cdot x_{i_2} y_{i_2} \cdot \dots \cdot x_{i_p} y_{i_p} \tag{20}$$

since the coupling constants are uncorrelated. Clearly R_{xy} depends only on the number of positions in which x and y differ, i.e., on the Hamming distance $d(x,y)$. As shown in (Weinberger and Stadler 1992) the autocorrelation function is

$$\rho(d) = R_{xy}/R_{xx} = \frac{1}{\binom{n}{p}} \sum_{l=0}^{n} (-1)^{\ell} \binom{d}{\ell} \binom{n-d}{p-\ell} = \frac{1}{\binom{n}{p}} \mathbf{K}^{(2)}_{n,p}(d) \tag{22}$$

where $\mathbf{K}^{(2)}_{n,p}$ is a Krawtchouk polynomial. These functions are widely used in coding theory (see e.g. vanLint 1982), and they are known to be the orthogonal polynomials associated with the Boolean Hypercube (Dunkl 1976, Koornwinder 1982). Therefore we have the following

Corollary. The autocorrelation function r of the p-spin model along a random walk is the exponential $r(s) = \lambda_p^s$ where $\lambda_p = 1 - 2p/n$ is the $p+1$-th eigenvalue of $\frac{1}{N(1)}C$. If n is even and $p = n/2$ we find an uncorrelated time series along a simple random walk. The simplest non-trivial model of this class, the Sherrington-Kirkpatrick model ($p = 2$), corresponds to the third eigenvalue of the intersection matrix.

A closely related model is the graph bipartitioning problem, obtained from the Sherrington-Kirkpatrick model by restricting the admissible configurations by $\sum_i x_i = 0$ (Fu and Anderson 1986). Neighbouring configuration differ by the spins in exactly two positions. The corresponding graph is distance transitive. Both $r(s)$ and $\rho(d)$ have been calculated exactly (Stadler and Happel 1992). The random walk autocorrelation function $r(s)$ is a decaying exponential related to the third eigenvalue of the intersection matrix.

Numerical calculations for the travelling salesman problem yield a decaying exponential autocorrelation function $r(s) \approx (1 - 4/n)^s$ for large n, if the graph Γ is chosen as the Cayley graph of the symmetric group with transpositions as the set of generators (Stadler and Schnabl 1992). Random walk on this graph have been studied by Diaconis and Shashahani (1981). Interestingly, for $n \geq 12$ the third eigenvalue of the corresponding transition matrix equals $(1 - 4/n)$.

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