

Almost-Orthogonal Bases for Inner Product Polynomials

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Abstract

In this paper, we consider low-degree polynomials of inner products between a collection of random vectors. We give an almost orthogonal basis for this vector space of polynomials when the random vectors are Gaussian, spherical, or Boolean. In all three cases, our basis admits an interesting combinatorial description based on the topology of the underlying graph of inner products.

We also analyze the expected value of the product of two polynomials in our basis. In all three cases, we show that this expected value can be expressed in terms of collections of matchings on the underlying graph of inner products. In the Gaussian and Boolean cases, we show that this expected value is always non-negative. In the spherical case, we show that this expected value can be negative but we conjecture that if the underlying graph of inner products is planar then this expected value will always be non-negative.

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1 Introduction

When we have a collection of random variables, it is often extremely useful to find a basis of polynomials in the random variables which is orthonormal under the natural inner product $\langle f, g \rangle := \mathbb{E}[f \cdot g]$. Some important examples are as follows:

1. If x is a random point of the Boolean hypercube $\{-1, 1\}^n$ then the multilinear monomials $\{\prod_{i \in S} x_i : S \subseteq [n]\}$ are an orthonormal basis.
2. When we have a single Gaussian variable $x \sim \mathcal{N}(0, 1)$, the Hermite polynomials (with the correct normalization) are an orthonormal basis. When x is an n -dimensional vector with Gaussian coordinates (i.e. $x \sim \mathcal{N}(0, \text{Id}_n)$), the multivariate Hermite polynomials form an orthonormal basis.
3. When $x \in \mathbb{R}^n$ is a random unit vector (i.e. $x \in_{\mathbb{R}} S^{n-1}$), spherical harmonics give an orthonormal basis.

In this paper, we consider polynomials of inner products between a collection of random vectors. More precisely, fix a finite set of vertices V and $n \in \mathbb{N}$ and consider drawing i.i.d. random n -dimensional vectors d_u for each $u \in V$. We will work in three settings: when the



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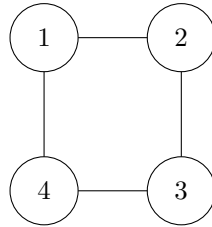
n -dimensional vector d_u is a standard Gaussian, a uniform unit vector, and a uniform Boolean vector. We consider polynomials in the variables $d_{u,i}$ with real coefficients which have degree less than n and are orthogonally invariant i.e. unchanged if the $\{d_u\}$ are simultaneously replaced by $\{Td_u\}$ for any orthogonal matrix T . Any such orthogonally invariant polynomial will also be expressible¹ in terms of the inner product variables $x_{uv} := \langle d_u, d_v \rangle$.

A natural spanning set for the space of orthogonally invariant polynomials is the set of monomials $\prod_{u,v \in V} x_{uv}^{k_{uv}}$ where each $k_{uv} \in \mathbb{N}$. Equivalently, there is one monomial for each undirected multigraph on V (with self-loops allowed in the Gaussian case): for the monomial $\prod_{u,v \in V} x_{uv}^{k_{uv}}$ we take the graph where there are k_{uv} multi-edges from u to v . We denote this monomial by m_G where G is the underlying graph.

However, the monomials m_G are not orthogonal. For example, one can check that in the Gaussian case, the graph shown in Figure 1 has

$$\mathbb{E}[x_{12}x_{23}x_{34}x_{41}] = \mathbb{E}_{d_1, d_2, d_3, d_4 \sim \mathcal{N}(0, \text{Id}_n)} [\langle d_1, d_2 \rangle \langle d_2, d_3 \rangle \langle d_3, d_4 \rangle \langle d_4, d_1 \rangle] = n.$$

Our goal in this paper is to orthogonalize the m_G into a basis of polynomials p_G . As it



■ **Figure 1** Four-cycle of inner products.

turns out, the basis p_G which we will obtain is not quite orthogonal, but it is very close. In particular, we will have that $\langle p_G, p_H \rangle = 0$ unless $V(G) = V(H)$ and G and H have the same degree at every vertex. In addition, even when $G \neq H$ and $\langle p_G, p_H \rangle \neq 0$, $\langle p_G, p_H \rangle$ will be small (see Lemma 63).

While the p_G basis is not quite orthogonal, it exhibits some surprisingly beautiful combinatorics based on the underlying graph G . Even computing $\mathbb{E}[m_G]$, one can already see a connection to the topology of the graph G . In the Gaussian case, the magnitude of $\mathbb{E}[m_G]$ is n^k where k is the maximum number of cycles that $E(G)$ can be partitioned into (and is 0 if G has a vertex with odd degree) and analogous results hold for the spherical and Boolean cases (see Lemma 11, Lemma 32, and Lemma 56). A theme of this paper is that quantities involving the m_G and p_G may not have clean exact formulas, but their magnitudes in n are determined by combinatorial and topological properties of G .

1.1 Outline

In the remainder of the introduction, we give more overview on the p_G in general. In Section 2 we specialize to the Gaussian case $d_u \sim \mathcal{N}(0, \text{Id}_n)$. In the Gaussian case, the calculations work out cleanly once one has the right definitions. In Section 3 we continue

¹ When d_u is a Boolean vector, we instead require that the polynomials are invariant under permutations of $[n]$ and changing the signs of coordinates (i.e. automorphisms of the Boolean hypercube). In this setting, in addition to inner products, we also have k -wise inner products for all even $k > 2$. For more details, see Section 4.

to the spherical case. Here the calculations become more involved, and we investigate a conjecture relating the spherical case to planar graphs. In Section 4 we investigate the Boolean case $d_u \in_{\mathbb{R}} \{-1, +1\}^n$ which combines aspects of the Gaussian and spherical cases. In Section 5 we give a “Fourier inversion” lemma for potential applications. For the purpose of gaining intuition about the family p_G , it may be helpful to carry around a few small examples and see how the results and proofs apply to these polynomials.

1.2 Constructing the polynomials

Given any inner product on polynomials, we can automatically construct an orthonormal basis of polynomials by using the Gram-Schmidt process. However, to run Gram-Schmidt, it is necessary to choose an order. A natural order for polynomials is by degree, though within each degree it is not clear how the polynomials should be ordered. We skirt this issue by only orthogonalizing a monomial against polynomials with lower degree². The resulting polynomials we produce are “mostly orthogonal”, with $\mathbb{E}[p_G \cdot p_H]$ possibly nonzero for polynomials of the same degree (in fact, they will be orthogonal unless G and H have the same degree on every vertex). We call this the *degree-orthogonal Gram-Schmidt process*.

► **Definition 1.** A polynomial family $\{p_I\}_{I \in \mathcal{I}}$ is degree-orthogonal (with respect to \mathcal{D}) if $\mathbb{E}_{d \sim \mathcal{D}}[p_I(d)p_J(d)] = 0$ whenever $\deg(p_I) \neq \deg(p_J)$.

The degree-orthogonal Gram-Schmidt process outputs the unique monic degree-orthogonal basis.

► **Fact 2 (Uniqueness of Gram-Schmidt orthogonalization).** Let $\{m_I\}_{I \in \mathcal{I}}$ be the set of monomials of degree at most τ in a set of variables ν and let \mathcal{D} be a distribution on \mathbb{R}^ν such that $\{m_I\}_{I \in \mathcal{I}}$ are linearly independent as functions on the support of \mathcal{D} . There is a unique set of monic polynomials $\{p_I\}_{I \in \mathcal{I}}$ such that

- (i) The unique monomial of maximum degree in p_I is m_I ,
- (ii) The family p_I is degree-orthogonal with respect to \mathcal{D} .

Furthermore, the p_I are linearly independent and span the same space as the m_I .

Proof. Condition (i) says that p_I lies in the space $\text{span}(\{m_I\} \cup \{m_J : \deg(m_J) < \deg(m_I)\})$. Condition (ii) says that p_I is orthogonal to the latter subspace of codimension 1, and therefore p_I is determined since it’s monic. ◀

► **Remark 3.** Our monomials $\{m_G\}$ are not linearly independent when the degree is too high. In this case, $\{p_G\}$ will be a spanning set rather than a basis.

However, Gram-Schmidt certainly does not guarantee any nice description of the resulting polynomials. It turns out that the p_G also have closed-form combinatorial descriptions and we now give one such description. However, calculations are still a pain using this description. In the next sections we will give alternate combinatorial formulas for the p_G based on collections of matchings that allow for calculations, and also highlight the connection between the p_G and the topology of the graph G .

Let $d \sim \mathcal{D}^{\otimes V}$ for some distribution \mathcal{D} on \mathbb{R}^n , which we will later take to be either Gaussian, uniformly spherical, or uniformly Boolean. We want to find an orthogonal polynomial basis for $\text{Aut}(\mathcal{D})$ -invariant functions. Let $\{\chi_\alpha : \alpha \in \mathbb{N}^n\}$ be the monic polynomial family on \mathbb{R}^n which is degree-orthogonal under \mathcal{D} (this is the orthogonal basis for entries of a single

² Degree of a polynomial in this paper always refers to total degree.

vector, e.g. the multivariate Hermite polynomials in the Gaussian case). We assume that we have a set $\{m_I\}_{I \in \mathcal{I}}$ of homogeneous polynomials in the $d_{u,i}$ which form a (not necessarily orthogonal) basis for the $\text{Aut}(\mathcal{D})$ -invariant functions up to a certain degree. For example, this can be the inner product functions $\prod_{u,v \in V} \langle d_u, d_v \rangle^{k_{uv}}$ in the Gaussian and spherical cases. Construct $\{p_I\}_{I \in \mathcal{I}}$ by applying to m_I the map (extending by linearity),

$$\prod_{u \in V} d_u^{\alpha_u} \mapsto \prod_{u \in V} \chi_{\alpha_u}(d_u).$$

In words, each monomial is replaced by the \mathcal{D} -orthogonal polynomial with that leading monomial. As shown by the following proposition, the p_I are monic, degree-orthogonal, and have the same degree as the corresponding m_I , so if the p_I are $\text{Aut}(\mathcal{D})$ -invariant then the p_I are a monic degree-orthogonal basis for the $\text{Aut}(\mathcal{D})$ -invariant functions, and hence equal the output of the Gram-Schmidt process on m_I .

► **Proposition 4.** *The polynomials $\{p_I\}_{I \in \mathcal{I}}$ are monic, satisfy $\deg(p_I) = \deg(m_I)$, and are degree-orthogonal.*

Proof. The degree is preserved by the map sending $d_u^\alpha \mapsto \chi_\alpha(d_u)$ and the leading coefficient is 1 since the χ_α are monic. Suppose that p_I, p_J have distinct degrees; then so do m_I, m_J . For each term in the expression $p_I p_J$, because m_I, m_J are homogeneous and have different degree, there must be $u \in V$ such that the degree in d_u differs between p_I, p_J . Because of degree-orthogonality of the χ_α , the expectation over d_u is zero. ◀

However, it's not clear that the new polynomials p_I have the desired $\text{Aut}(\mathcal{D})$ symmetry without more assumptions on \mathcal{D} . For our settings we will check that this is indeed the case.

1.3 Related work

Some of the combinatorics of the monomials m_G is captured by the *circuit partition polynomial* [1] (see also the *Martin polynomial* [10, 5]) which is the univariate generating function for circuit partitions of G :

$$r_G(x) = \sum_{k \geq 0} r_k(G) x^k$$

where $r_k(G)$ is the number of ways to split the edges of G into exactly k circuits. $r_G(n) = \mathbb{E}[m_G]$ for the Gaussian distribution, as we show in Lemma 11. This formula was also computed by Moore and Russell [11], who also prove the spherical case, Lemma 32.

Although Gram-Schmidt works well for univariate polynomials, in general finding an *explicit* orthogonal basis of polynomials for a given space is a difficult task. Examples include polynomials on the unit ball and simplex [3] or a slice of the hypercube [6]. Occasionally it is simpler to find a degree-orthogonal family, as we do here. For example, “the” spherical harmonics (as originally given by Laplace in $n = 3$ dimensions, see Chapter 4 of [4] for general n) are an orthogonal basis for functions on the sphere. However, it is easier to use the “Maxwell representation”, which is only degree-orthogonal, as we do in Section 3.

To the best of our knowledge, the p_G have not been explored before. We now compare the p_G with several similar families of polynomials.

When G equals k multiedges between two vertices 1 and 2, p_G generalizes a univariate orthogonal polynomial family evaluated on $\langle d_1, d_2 \rangle$. For the spherical case this is the Gegenbauer polynomials. For the Boolean case, this is the Kravchuk polynomials (after an

affine shift). For the Gaussian case, p_G also depends on $\|d_1\|$ and $\|d_2\|$, but evaluated on $\langle d_1, d_1 \rangle = \langle d_2, d_2 \rangle = n$ this is the (probabilist's) Hermite polynomials.

For a collection of jointly Gaussian random variables X_i , the *Wick product* gives a monic orthogonal polynomial family under the expectation inner product [9]. In our set-up, there are two differences with the Wick product. First, the variables x_{uv} are not themselves Gaussian; they are individually distributed as $\sqrt{X} \cdot Y$ where X is a chi-squared random variable with n degrees of freedom and Y is an independent standard Gaussian. This however could be fixed by using bipartite graphs G and sampling d_u as a Gaussian vector on one bipartition and as a spherical vector on the other. The second and more important difference is that even if this change is made, the x_{uv} are individually Gaussian but not jointly Gaussian. The graph structure of G enforces nontrivial correlations. For example, in the four-cycle given earlier in Figure 1, each edge is mean-zero and each pair of edge variables is uncorrelated, and so if the variables were jointly Gaussian then they would be independent and mean-zero. However, $\mathbb{E}[x_{12}x_{23}x_{34}x_{14}] > 0$.

The *matching polynomial* of a graph G is the univariate generating function for the number of matchings in G . Despite both families generalizing e.g. the Hermite polynomials, the matching polynomials and p_G seem incomparable.

For a permutation group $G \leq S_k$, one defines the *cycle polynomial* [2]

$$\sum_{g \in G} x^{\text{number of cycles in } g}.$$

Though this is similar in appearance to some calculations in this paper, there is not a clear group G associated with the matching structures that we consider.

1.4 Applying the p_G basis

We end the introduction by describing how the p_G basis may be applied. The p_G basis behaves like a Fourier basis for orthogonally invariant functions of a collection of vectors $d = \{d_u\}$. While other bases may be simpler, the p_G basis is specialized to orthogonally invariant functions and it exhibits nontrivial combinatorial cancellations which would be hard to spot and explain in other bases, and which might be intrinsic to some problems. We expect that the p_G will be most useful for applications where we work with large n and relatively low-degree moments of \mathcal{D} , such as analyzing the sum of squares hierarchy or the trace power method at low degrees.

We encountered the p_G basis in the course of the work [7], in which a superset of the current authors prove lower bounds against the sum of squares hierarchy for the Sherrington-Kirkpatrick problem. Technically, this work constructs a matrix \mathcal{M} which is a function of a collection of random Gaussian vectors $\{d_u\}$; the entries of \mathcal{M} are naturally expressed (via “pseudocalibration”) in terms of an orthogonal polynomial basis evaluated on the d_u . Ultimately, we ended up using the standard Hermite basis as this was sufficient for our purposes, though we also considered using the p_G basis.

2 Polynomial Basis for the Gaussian Setting

In this section we investigate the family $\{p_G\}$ when $d_u \sim \mathcal{N}(0, \text{Id}_n)$ i.i.d. The graph G is a multigraph on V , possibly with self-loops. We will develop a combinatorial understanding of the polynomials through “routings” (Definition 14) and use it to give formulas for the inner product (Lemma 23) and variance (Corollary 25).

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Note that the m_G are not completely linearly independent. For example, if $n = 1$, then m_G is determined by its degrees on each vertex. Despite this, the low-degree monomials are linearly independent.

► **Lemma 5.** *The set of m_G for $|E(G)| \leq n$ is linearly independent.*

Proof. Suppose that $\sum_{G:|E(G)| \leq n} c_G m_G = 0$; we show $c_G = 0$. Each inner product $\langle d_u, d_v \rangle$ can be expanded as $\sum_{i=1}^n d_{u,i} d_{v,i}$. In this way, each edge gets a label from 1 to n . Expanding m_G ,

$$m_G = \sum_{\sigma: E(G) \rightarrow [n]} \prod_{\{u,v\} \in E(G)} d_{u,\sigma(\{u,v\})} d_{v,\sigma(\{u,v\})}.$$

Since $|E(G)| \leq n$, one monomial that appears in m_G will have σ assign a distinct label to each edge. We claim that this monomial appears in the sum with coefficient c_G : because the edge labels are distinct, we can recover the graph G from the monomial. Therefore $c_G = 0$. ◀

For low-degree polynomials the p_G will therefore be a basis.

The polynomials p_G admit several nice combinatorial descriptions based on the graph G . To see why something combinatorially nice might be expected to happen, there is a combinatorially-flavored method for computing $\mathbb{E}[m_G]$ via Isserlis' theorem (also known as Wick's lemma).

► **Lemma 6 (Isserlis' theorem).** *Fix vectors $d_1, \dots, d_{2k} \in \mathbb{R}^n$. Then for v a standard n -dimensional Gaussian random variable,*

$$\mathbb{E}_v[\langle v, d_1 \rangle \cdots \langle v, d_{2k} \rangle] = \sum_{\substack{\text{perfect matchings } (u,v) \in M \\ M \text{ on } [2k]}} \prod \langle d_u, d_v \rangle.$$

Observe also that the expectation is zero when there are an odd number of inner products.

We will need the following minor generalization.

► **Lemma 7.** *For fixed $d_1, \dots, d_{2k} \in \mathbb{R}^n$ and $v \sim \mathcal{N}(0, Id_n)$,*

$$\mathbb{E}_v[\langle v, v \rangle^{2l} \langle v, d_1 \rangle \cdots \langle v, d_{2k} \rangle] = n(n+2) \cdots (n+2l-2) \sum_{\substack{\text{perfect matchings } (u,v) \in M \\ M \text{ on } [2k]}} \prod \langle d_u, d_v \rangle.$$

Proof. See the full version of the paper. ◀

The generalization can be iterated to compute $\mathbb{E}[m_G]$ for a given graph G . We take the expectation over the vectors d_u one at a time, and each application reduces our expression to a sum over graphs that no longer involve u .

To capture the combinatorics of the p_G , we look at matchings of the edge endpoints incident to a given vertex. More specifically we use a collection M of (partial or perfect) matchings on incident edges, one for each vertex.

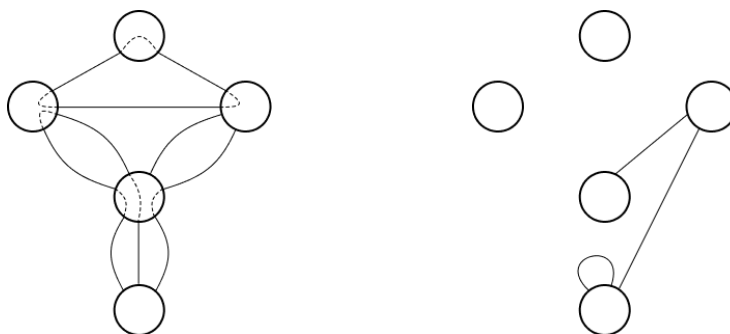
► **Definition 8.** *Let $\mathcal{PM}(G)$ be the set of all perfect matching collections of the edges incident to each vertex of G . Each element of $\mathcal{PM}(G)$ specifies $|V(G)|$ perfect matchings, and the perfect matching for vertex v is on $\deg(v)$ elements.*

Let $\mathcal{M}(G)$ denote the set of all partial or perfect matching collections of the edges incident to each vertex of G .

► **Definition 9.** For $M \in \mathcal{M}(\mathcal{G})$, define the routed graph $\text{route}(M)$ to be the graph obtained by connecting up edge endpoints that are matched at each vertex v . Closed cycles are deleted, and paths are replaced by a single edge between the final path endpoints.

► **Definition 10.** For $M \in \mathcal{M}(\mathcal{G})$, define $\text{cycles}(M)$ to be the number of closed cycles formed by routing.

We give an example in Figure 2. The graph on the left has 5 vertices, and 10 edges denoted by solid lines. The edges are partially matched up at each vertex using the dashed edges. The right side shows the result of routing. $\text{cycles}(M) = 1$ and one closed cycle, the triangle, was deleted.



■ **Figure 2** Left: Unrouted graph with dashed edges denoting the partial matching collection. Right: Result of routing.

Using these definitions, we have the following formula for the expectation $\mathbb{E}[m_G]$,

► **Lemma 11.** $\mathbb{E}[m_G] = 0$ if some vertex in G has odd degree. Otherwise,

$$\mathbb{E}[m_G] = \sum_{M \in \mathcal{PM}(G)} n^{\text{cycles}(M)}.$$

Proof. Expanding m_G and grouping by vertex,

$$m_G = \sum_{\sigma: E \rightarrow [n]} \prod_{u \in V, i \in [n]} d_{u,i}^{\#\{e \ni u : \sigma(e)=i\}}.$$

Taking expectations, the $d_{u,i}$ are independent Gaussians. If one of the vertices has odd degree, one of the labels i will necessarily occur an odd number of times at that vertex and the overall expectation will be zero. Otherwise, $\mathbb{E}[Z^{2k}] = (2k - 1)!!$ for $Z \sim \mathcal{N}(0, 1)$. The expression $(2k - 1)!!$ counts the number of perfect matchings of $2k$ elements; in this case when computing $\mathbb{E}[d_{u,i}^{\#\{e \ni u : \sigma(e)=i\}}]$ these should be thought of as summing 1 for each perfect matching of the edges incident to u which are labeled i . In summary, each σ sums over a subset of \mathcal{PM} .

Now fix a given collection of perfect matchings $M \in \mathcal{PM}$; which σ contribute to it? We require that, at each vertex, every pair of endpoints matched in M are assigned the same label. Therefore, in any cycle formed by $\text{route}(M)$, the labeling σ must assign all edges of the cycle the same label. These labels can be any number from $[n]$, and disjoint cycles don't affect each other. Therefore there are $n^{\text{cycles}(M)}$ such σ . ◀

► **Corollary 12.** The magnitude of $\mathbb{E}[m_G]$ is n^k where k is the maximum number of cycles into which $E(G)$ can be partitioned (note that this is NP-hard to compute from G).

We now give several alternate definitions of the polynomials p_G .

► **Definition 13** (Hermite sum definition). Define p_G by

$$p_G = \sum_{\sigma: E(G) \rightarrow [n]} \prod_{u \in V, i \in [n]} h_{|\{e \ni u : \sigma(e)=i\}|}(d_{u,i}).$$

Note that in this definition we consider a self-loop at u labeled i to contribute 2 to $|\{e \ni u : \sigma(e) = i\}|$.

► **Definition 14** (Routing definition). Define p_G by

$$p_G = \sum_{M \in \mathcal{M}(G)} m_{\text{route}(M)} \cdot n^{\text{cycles}(M)} \cdot (-1)^{|M|}.$$

A given graph K can appear as $\text{route}(M)$ for several different matchings M (even with different numbers of cycles). This gives rise to interesting and nontrivial coefficients on the monomials m_K .

► **Definition 15** (Generic construction from Proposition 4). Consider the Hermite expansion of m_G in the variables $d_{u,i}$, and let p_G be the truncation to the top level i.e. keep only those Hermite coefficients $c_\alpha h_\alpha$ with $|\alpha| = 2|E(G)|$.

Since m_G is homogeneous as a function of the $d_{u,i}$ and each monomial appears with coefficient 1, this amounts to taking each monomial d^α and replacing it by $h_\alpha(d)$.

► **Lemma 16.** The three definitions above are equivalent.

Proof. After checking that the leading monomial of p_G in Definition 13 is m_G , it is clear that Definition 13 and Definition 15 are equivalent.

We argue Definition 13 and Definition 14 agree. The coefficient of x^{k-2i} in the Hermite polynomial $h_k(x)$ can be interpreted as the number of matchings of $2i$ objects out of k total (there is also an alternating sign). In this way h_k is a generating function for all partial matchings on $[k]$. Looking at $h_{|\{e \ni u : \sigma(e)=i\}|}(d_{u,i})$, we interpret this (ignoring the sign for now) as summing over all partial matchings on the incident edges with a given label i ; any matched edges are given a factor of 1 while the unmatched edges are given $d_{u,i}$.

Now look at the view from a given collection M of partial matchings, one per vertex. Which σ contribute? Along any closed cycle in $\text{route}(M)$, the labels σ must be all the same, and if this is the case the contribution is 1. Along any path, the labels assigned by σ must also be the same, say i . The multiplicative contribution of any interior vertices is 1, but the contribution of the two endpoint vertices u and v is $d_{u,i}$ and $d_{v,i}$. When all valid σ are summed over, we obtain a factor of n for each cycle, and the inner product between the endpoints of each path.

The $(-1)^{|M|}$ factor comes from the signings of the Hermite coefficients. ◀

► **Example 17.** Let G be the graph with vertices $V(G) = \{u, v_1, v_2, v_3\}$ and edges $E(G) = \{\{u, v_1\}, \{u, v_2\}, \{u, v_3\}\}$. We have that

$$\begin{aligned} m_G &= \langle d_u, d_{v_1} \rangle \langle d_u, d_{v_2} \rangle \langle d_u, d_{v_3} \rangle \\ &= \sum_{\text{distinct } i, j, k \in [n]} d_{u,i} d_{u,j} d_{u,k} d_{v_1,i} d_{v_2,j} d_{v_3,k} + \sum_{i \neq j \in [n]} d_{u,i}^2 d_{u,j} d_{v_1,i} d_{v_2,i} d_{v_3,j} \\ &+ \sum_{i \neq j \in [n]} d_{u,i}^2 d_{u,j} d_{v_1,i} d_{v_2,j} d_{v_3,i} + \sum_{i \neq j \in [n]} d_{u,i}^2 d_{u,j} d_{v_1,j} d_{v_2,i} d_{v_3,i} + \sum_{i \in [n]} d_{u,i}^3 d_{v_1,i} d_{v_2,i} d_{v_3,i}. \end{aligned}$$

Replacing the monomial $d_{u,i}^2$ with the corresponding Hermite polynomial $d_{u,i}^2 - 1$ and replacing the monomial $d_{u,i}^3$ with the corresponding Hermite polynomial $d_{u,i}^3 - 3d_{u,i}$, we have that

$$\begin{aligned} p_G &= \sum_{\text{distinct } i,j,k \in [n]} d_{u,i} d_{u,j} d_{u,k} d_{v_1,i} d_{v_2,j} d_{v_3,k} + \sum_{i \neq j \in [n]} (d_{u,i}^2 - 1) d_{u,j} d_{v_1,i} d_{v_2,i} d_{v_3,j} \\ &+ \sum_{i \neq j \in [n]} (d_{u,i}^2 - 1) d_{u,j} d_{v_1,i} d_{v_2,j} d_{v_3,i} + \sum_{i \neq j \in [n]} (d_{u,i}^2 - 1) d_{u,j} d_{v_1,j} d_{v_2,i} d_{v_3,i} \\ &+ \sum_{i \in [n]} (d_{u,i}^3 - 3d_{u,i}) d_{v_1,i} d_{v_2,i} d_{v_3,i} \end{aligned}$$

The term $-d_{u,j} d_{v_1,i} d_{v_2,i} d_{v_3,j}$ and one of the 3 terms $-d_{u,i} d_{v_1,i} d_{v_2,i} d_{v_3,i}$ correspond to the collection of matchings M where v_1 is matched to v_2 at u (and all other matchings are trivial). Summing these terms over all $i \neq j \in [n]$ gives $-\langle d_{v_1}, d_{v_2} \rangle \langle d_u, d_{v_3} \rangle$.

Similarly, the term $-d_{u,j} d_{v_1,i} d_{v_2,j} d_{v_3,i}$ and one of the 3 terms $-d_{u,i} d_{v_1,i} d_{v_2,i} d_{v_3,i}$ correspond to the collection of matchings M where v_1 is matched to v_3 at u (and all other matchings are trivial). Summing these terms over all $i \neq j \in [n]$ gives $-\langle d_{v_1}, d_{v_3} \rangle \langle d_u, d_{v_2} \rangle$.

Finally, the term $-d_{u,j} d_{v_1,j} d_{v_2,i} d_{v_3,i}$ and one of the 3 terms $-d_{u,i} d_{v_1,i} d_{v_2,i} d_{v_3,i}$ correspond to the collection of matchings M where v_2 is matched to v_3 at u (and all other matchings are trivial). Summing these terms over all $i \neq j \in [n]$ gives $-\langle d_{v_2}, d_{v_3} \rangle \langle d_u, d_{v_1} \rangle$.

Putting everything together,

$$p_G = \langle d_u, d_{v_1} \rangle \langle d_u, d_{v_2} \rangle \langle d_u, d_{v_3} \rangle - \langle d_{v_1}, d_{v_2} \rangle \langle d_u, d_{v_3} \rangle - \langle d_{v_1}, d_{v_3} \rangle \langle d_u, d_{v_2} \rangle - \langle d_{v_2}, d_{v_3} \rangle \langle d_u, d_{v_1} \rangle.$$

As a consequence of the routing definition we have

► **Lemma 18.** *The polynomials p_G are orthogonally invariant.*

► **Corollary 19.** *Definitions 13, 14, 15 are equal to the degree-orthogonal Gram-Schmidt process on m_G .*

Proof. From Proposition 4, the polynomials defined above are degree-orthogonal and monic. The previous lemma shows that they are orthogonally invariant. Therefore they match the result of Gram-Schmidt by Fact 2. ◀

In fact, the proof of Proposition 4 shows that p_G have a stronger ‘‘ultra-orthogonality’’ property. If G and H have different degree at u , then only taking the expectation over d_u already results in the zero polynomial.

► **Lemma 20.** *Let G and H be two multigraphs. If $\deg_G(u) \neq \deg_H(u)$ for some $u \in V$,*

$$\mathbb{E}_{d_u \sim \mathcal{N}(0, Id_n)} [p_G \cdot p_H] = 0.$$

We now derive an explicit formula for the inner product and variance of p_G . For two graphs G, H on V , we define $G \cup H$ to be the disjoint union of the edges (the edge multiplicity in $G \cup H$ is the sum of the multiplicities in G and H).

► **Definition 21.** *For two multigraphs, write $G \leftrightarrow H$ if $\deg_G(u) = \deg_H(u)$ for all $u \in V$.*

► **Definition 22.** *Let $\mathcal{PM}(G, H) \subseteq \mathcal{PM}(G \cup H)$ be perfect matching collections such that at each vertex v , the matching goes between edges incident to v in G and edges incident to v in H . Note that if $G \not\leftrightarrow H$, then $\mathcal{PM}(G, H)$ is empty.*

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► **Lemma 23.** *Let G and H be two multigraphs.*

$$\mathbb{E}[p_G \cdot p_H] = \sum_{M \in \mathcal{PM}(G, H)} n^{\text{cycles}(M)}$$

► **Remark 24.** Determining the maximum number of cycles in $M \in \mathcal{PM}(G, H)$ is NP-hard via a slight modification of [8]. This remains true if we restrict the cycles to be simple.

Proof. Use the routing definition of p_H ,

$$p_G \cdot p_H = \sum_{\substack{M_1 \in \mathcal{M}(G), \\ M_2 \in \mathcal{M}(H)}} m_{\text{route}_G(M_1)} \cdot m_{\text{route}_H(M_2)} \cdot n^{\text{cycles}_G(M_1) + \text{cycles}_H(M_2)} \cdot (-1)^{|M_1| + |M_2|}.$$

Taking expectations, by Lemma 11 we sum over all perfect matchings of $\text{route}_G(M_1) \cup \text{route}_H(M_2)$ which “complete” the partial matchings M_1 and M_2 , when viewed as a matching on the graph $G \cup H$. The power of n is the number of cycles in the completed matching. The net effect is to sum over all perfect matching collections in $G \cup H$,

$$\mathbb{E} p_G p_H = \sum_{M \in \mathcal{PM}(G \cup H)} n^{\text{cycles}_{G \cup H}(M)} \sum_{\text{pick some } M\text{-matched pairs to be in } M_1 \text{ or } M_2} (-1)^{|M_1| + |M_2|}.$$

The inner summation often cancels to zero. In the graph $G \cup H$, each edge-vertex incidence comes from either G or H . We can only add an M -matched pair to M_1 if both matched edge-vertex incidences come from G ; similarly only matched pairs which are both in H can be picked for M_2 . If there are any such pairs, the inner summation is automatically zero.

The remaining terms are those M in which, at every vertex, the perfect matching is a perfect matching between incoming edges in G and those in H – that is, matching collections in $\mathcal{PM}(G, H)$. For these terms, the inner summation is trivially 1, which finishes the proof. ◀

► **Corollary 25.** $n^{|E(G)|} \leq \mathbb{E}[p_G^2] \leq |E(G)|^{2|E(G)|} \cdot n^{|E(G)|}$.

Proof. Using the result of Lemma 23, we claim $\max_{M \in \mathcal{PM}(G, G)} \text{cycles}(M) = |E(G)|$. On the one hand, $|E(G)|$ is achievable by matching each edge with its duplicate to create 2-cycles. On the other hand, every cycle in $\text{route}(M)$ needs at least two edges (there can be no self-loops as matchings with self-loops are not in $\mathcal{PM}(G, G)$). This shows $n^{|E(G)|} \leq \mathbb{E} p_G^2 \leq |\mathcal{PM}(G, G)| \cdot n^{|E(G)|}$.

$\mathcal{PM}(G, G)$ consists of choosing a perfect matching at each vertex between two sets of size $\deg(v)$.

$$|\mathcal{PM}(G, G)| = \prod_{v \in V} \deg(v)! \leq |E(G)|^{2|E(G)|}.$$

3 Polynomial Basis for the Spherical Setting

Let $S^{n-1} = \{x \in \mathbb{R}^n : \|x\|_2 = 1\}$. With the d_u drawn uniformly and independently from S^{n-1} instead of the Gaussian distribution, for each multigraph G with no self-loops (reflecting the fact that $\langle d_u, d_u \rangle = 1$) we construct a polynomial p_G . We again construct the polynomials in terms of routings (Definition 35) and study the inner product (Section 3.1) and variance (Corollary 43). For the most part, the proofs in this section mirror their counterparts in the

previous section, with the notable exception of the inner product formula, which exhibits surprising mathematical depth.

Let $\alpha \in \mathbb{N}^n$ be a multi-index and $|\alpha| := \sum_{i=1}^n \alpha_i$. We will need the Maxwell representation of harmonic polynomials [3, Theorem 1.1.9]. Concretely, let the spherical harmonic $s_\alpha : S^{n-1} \rightarrow \mathbb{R}$ be (the restriction to S^{n-1} of the function on \mathbb{R}^n)

$$s_\alpha(x) = \|x\|^{2|\alpha|+n-2} \frac{\partial}{\partial x^\alpha} \|x\|^{-n+2}$$

and then scaled to be monic. An alternate method to write down s_α is to first write down the Hermite polynomial $\prod_{i=1}^n h_{\alpha_i}(x_i)$ and then multiply each non-leading monomial of total degree $|\alpha| - 2k$ by approximately³ n^{-k} . More precisely, we let $x^{\underline{k}}$ be notation for the “fall-by-2” falling factorial,

$$x^{\underline{k}} := x(x-2)(x-4) \cdots (x-2k+2),$$

and let $x^{\overline{-k}} := 1/x^{\underline{k}}$. We also define $x^{\overline{k}}$ likewise for rise-by-2. Then:

► **Fact 26.** *To form s_α from h_α , multiply monomials with degree $|\alpha| - 2k$ by $(n + 2|\alpha| - 4)^{\overline{-k}}$.*

We will need the moments of the uniform distribution on the sphere (using the notation introduced above):

► **Fact 27.**

$$\mathbb{E}_{x \in_R S^{n-1}} [x^\alpha] = \begin{cases} n^{\overline{-|\alpha|/2}} \cdot \mathbb{E}_{Z \sim \mathcal{N}(0, Id_n)} [Z^\alpha] & \text{If } \alpha_i \text{ even for all } i \\ 0 & \text{Otherwise} \end{cases}$$

These spherical harmonics are degree-orthogonal (as functions of a single vector):

► **Fact 28.** *If $|\alpha| \neq |\beta|$, then $\mathbb{E}_{x \in_R S^{n-1}} [s_\alpha(x)s_\beta(x)] = 0$.*

We remark that $\{s_\alpha : \alpha \in \mathbb{N}^n\}$ is not completely linearly independent as functions on S^{n-1} because of the identity $\langle v, v \rangle = 1$:

► **Fact 29.** *For each k , the set $\{s_\alpha : |\alpha| \leq k, \alpha_n = 0 \text{ or } 1\}$ is a basis for the set of degree- $(\leq k)$ polynomial functions on S^{n-1} . The same holds for the monomials x^α .*

The monomials m_G are defined as before for each multigraph on V without self-loops. They are not completely linearly independent as functions on $(S^{n-1})^V$. We restrict ourselves to the set of low-degree functions, which are linearly independent.

► **Lemma 30.** *The set of m_G with $|E(G)| \leq n - 1$ is linearly independent as functions on $(S^{n-1})^V$.*

Proof. Suppose $\sum_{G: |E(G)| \leq n} c_G m_G = 0$ where c_G are not all zero, and let G be a nonzero graph with maximum number of edges. Expanding m_G ,

$$m_G = \sum_{\sigma: E(G) \rightarrow [n]} \prod_{\{u,v\} \in E(G)} d_{u,\sigma(\{u,v\})} d_{v,\sigma(\{u,v\})}.$$

³ Multiplying the monomials by exactly n^{-k} creates polynomials orthogonal under the distribution $\mathcal{N}(0, Id_n/n)$, which is similar to the unit sphere.

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Letting σ be an injective assignment of labels from $[n-1]$ (which exists because $|E(G)| \leq n-1$), we claim that the corresponding monomial, which we call the “special monomial”, is uncanceled and appears with coefficient c_G .

First, the relations $\langle d_u, d_u \rangle = 1$ mean that polynomials do not have a unique representation as functions on $(S^{n-1})^V$. We amend this by using the relations to reduce the degree of variable $d_{u,n}$ to 0 or 1 for each vertex u , replacing $d_{u,n}^2 = 1 - \sum_{i=1}^{n-1} d_{u,i}^2$. Nothing needs to be done for the special monomial.

After performing the replacement, the special monomial still does not arise from any other graphs. This is because the reduction step must either lower the degree, or introduce a variable with degree 2, whereas the special monomial is multilinear and was chosen to have maximum degree. Therefore, the special monomial has coefficient c_G , which is nonzero, a contradiction. \blacktriangleleft

There is a spherical Isserlis theorem which gives a recursive method to compute $\mathbb{E}[m_G]$.

► **Lemma 31** (Spherical Isserlis theorem). *Fix vectors $d_1, \dots, d_{2k} \in \mathbb{R}^n$. Then for $v \in_R S^{n-1}$,*

$$\mathbb{E}_v[\langle v, d_1 \rangle \cdots \langle v, d_{2k} \rangle] = n^{-\overline{k}} \sum_{\substack{\text{perfect matchings} \\ \mathcal{M} \text{ on } [2k]}} \prod_{(u,v) \in \mathcal{M}} \langle d_u, d_v \rangle.$$

Observe also that the expectation is zero when there are an odd number of inner products.

Proof. This follows from the standard Isserlis theorem. Let $Q \sim \chi^2(n)$ be a chi-square random variable with n degrees of freedom, independent from v . Then

$$\mathbb{E}_{v,Q}[\langle \sqrt{Q}v, d_1 \rangle \cdots \langle \sqrt{Q}v, d_{2k} \rangle] = \mathbb{E}_{Z \sim \mathcal{N}(0, \text{Id}_n)}[\langle Z, d_1 \rangle \cdots \langle Z, d_{2k} \rangle].$$

Factoring out Q^k , the left-hand side is

$$\mathbb{E}_{v,Q}[\langle \sqrt{Q}v, d_1 \rangle \cdots \langle \sqrt{Q}v, d_{2k} \rangle] = \mathbb{E}_Q[Q^k] \cdot \mathbb{E}_v[\langle v, d_1 \rangle \cdots \langle v, d_{2k} \rangle] = n^{\overline{k}} \mathbb{E}_v[\langle v, d_1 \rangle \cdots \langle v, d_{2k} \rangle].$$

By the Gaussian Isserlis theorem, the right-hand side equals

$$\mathbb{E}_{Z \sim \mathcal{N}(0, \text{Id}_n)}[\langle Z, d_1 \rangle \cdots \langle Z, d_{2k} \rangle] = \sum_{\substack{\text{perfect matchings} \\ \mathcal{M} \text{ on } [2k]}} \prod_{(u,v) \in \mathcal{M}} \langle d_u, d_v \rangle.$$

Dividing by $n^{\overline{k}}$ proves the claim. \blacktriangleleft

We also have explicit formulas based on matching collections,

► **Lemma 32.** $\mathbb{E}[m_G] = 0$ if there is a vertex of odd degree, otherwise,

$$\mathbb{E}[m_G] = \prod_{v \in V} n^{-\overline{\deg(v)/2}} \sum_{M \in \mathcal{PM}(G)} n^{\text{cycles}(M)}.$$

Proof. The proof goes through exactly as in the Gaussian case except that we plug in the spherical moments which contribute the rising factorial terms. \blacktriangleleft

► **Remark 33.** Lemma 32 is still valid if G has self-loops.

We now give three definitions of the orthogonal polynomials for the spherical case which are analogous to Definitions 13, 14, and 15 for the Gaussian case:

► **Definition 34** (Spherical harmonic sum definition). Define p_G by

$$p_G = \sum_{\sigma: E(G) \rightarrow [n]} \prod_{u \in V} s_{\text{histogram of } \{\sigma(e): e \ni u\}}(d_u).$$

► **Definition 35** (Routing definition). Define p_G by

$$p_G = \sum_{M \in \mathcal{M}(G)} m_{\text{route}(M)} \cdot n^{\text{cycles}(M)} \cdot (-1)^{|M|} \cdot \prod_{v \in V} (n + 2 \deg(v) - 4)^{\frac{-|M_v|}{2}}$$

where M_v is the partial matching of incident edges at v .

► **Definition 36** (Generic construction from Proposition 4). To construct p_G , expand the function m_G in the basis of spherical harmonics as a function of $d_{u,i}$ then truncate to the top-level coefficients of degree $2|E(G)|$.

► **Lemma 37.** The three definitions above are equivalent.

Proof. Definitions 34 and 36 agree once we check that the leading monomial in Definition 34 is m_G .

Definitions 34 and 35 agree as a consequence of equality between Definition 13 and Definition 14 in the Gaussian case by the following argument. For reference, we recall the two equal formulas for p_G in the Gaussian case,

$$p_G = \sum_{\sigma: E(G) \rightarrow [n]} \prod_{u \in V, i \in [n]} h_{|\{e \ni u : \sigma(e)=i\}|}(d_{u,i}) \quad (1)$$

$$p_G = \sum_{M \in \mathcal{M}(G)} m_{\text{route}(M)} \cdot n^{\text{cycles}(M)} \cdot (-1)^{|M|}. \quad (2)$$

For each fixed $\delta \in V^{\mathbb{N}}$, let us restrict to only the monomials in the variables $d_{u,i}$ with total degree $\delta(u)$ on the variables $\{d_{u,i} : i \in [n]\}$. We clearly still have equality between Equation (1) and Equation (2) after making this restriction. The equality still holds if we multiply both sides by an appropriate function of n ; we choose this function of n to be the product that appears on the right side of Definition 35, which only depends on δ . This clearly converts Equation (2) into Definition 35. Due to the choice of function, it also turns Equation (1) into Definition 34 because of the conversion between h_α and s_α in Fact 26. ◀

The following properties follow directly as they did in the Gaussian case:

► **Lemma 38.** The polynomials p_G are orthogonally invariant.

► **Lemma 39.** Let G and H be two multigraphs. If $\deg_G(u) \neq \deg_H(u)$ for some $u \in V$, then $\mathbb{E}_{d_u \in \mathbb{R}S^{n-1}}[p_G \cdot p_H] = 0$.

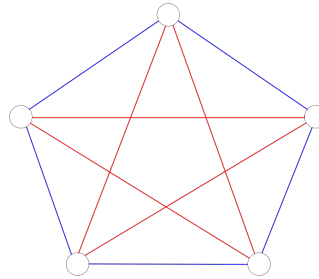
► **Lemma 40.** Definitions 34, 35, 36 are equal to the output of the degree-orthogonal Gram-Schmidt process on m_G .

3.1 Inner product

Unfortunately, we do not have a clean formula for the inner product of two spherical polynomials. Compared to the Gaussian case, there are several complications. First, in the spherical case some polynomials with $G \leftrightarrow H$ are orthogonal (whereas in the Gaussian case p_G and p_H are orthogonal iff $G \not\leftrightarrow H$, via Lemma 23). For example, the following two polynomials are orthogonal:

$$p_G = x_{12}x_{13}x_{45} - \frac{x_{23}x_{45}}{n}, \quad p_H = x_{14}x_{15}x_{23} - \frac{x_{45}x_{23}}{n}.$$

This shows that extra cancellations occur in the spherical case. Second, when n is small some of the p_G are degenerate. For example, if G is a triangle and $n = 2$ then $p_G = 0$. Third, even in the asymptotic regime of large n and constant-size graphs, in the spherical case the inner product may be negative (whereas in the Gaussian case the inner product is always non-negative). For example, this occurs if $E(G), E(H)$ partition the edges of K_5 , with the inner 5-cycle in G and the outer 5-cycle in H , as in Figure 3.



■ **Figure 3** Example of two graphs with negative inner product in the spherical case.

In this case it can be computed (see the full version of the paper) that

$$\mathbb{E}[p_G \cdot p_H] = \frac{-8(n-1)(n-2)(n-4)}{n^8(n+2)^4}.$$

Interestingly, we conjecture that negative inner product can only occur if the graph $G \cup H$ is nonplanar.

To attack these complications, we first give a general expression for the inner product. We use it to upper bound the magnitude of the inner product, showing that it's no larger than the Gaussian case, up to normalization (Corollary 44). In the full version of the paper, we study some situations when cancellations occur in an effort to determine the exact magnitude in n of the inner product.

The proof strategy we use is to consider the contribution c_M from each matching collection $M \in \mathcal{PM}(G \cup H)$ and then isolate cancellations that occur between these terms (similarly to how the inner product was computed in the Gaussian case, Lemma 23).

► **Definition 41.** For some $M \in \mathcal{PM}(G \cup H)$, define a G -pair as a pair of matched endpoints in M where both come from G . An H -pair and a (G, H) -pair are defined analogously.

Let $g_M(v)$ denote the number of G -pairs at vertex v and g_M denote the total number of G -pairs.

If $G \not\leftrightarrow H$ then $\mathbb{E}[p_G p_H] = 0$ by Lemma 39, so we may assume $G \leftrightarrow H$.

► **Lemma 42.** *Let G, H be arbitrary multigraphs such that $G \leftrightarrow H$. Let $d(v) = \deg_G(v) = \deg_H(v)$. Then*

$$\mathbb{E}[p_G \cdot p_H] = \prod_{v \in V} n^{\overline{-d(v)}} \sum_{M \in \mathcal{PM}(G \cup H)} c_M$$

where the coefficients c_M are

$$c_M = n^{\text{cycles}(M)} \prod_{v \in V} \frac{(-2)^{\overline{g_M(v)}}}{(n + 2d(v) - 4)^{\overline{g_M(v)}}}.$$

Proof. By orthogonality, $\mathbb{E}[p_G \cdot p_H] = \mathbb{E}[p_G \cdot m_H]$. Using the routing definition,

$$p_G \cdot m_H = \sum_{M \in \mathcal{M}(G)} m_{\text{route}_G(M)} \cdot m_H \cdot n^{\text{cycles}_G(M)} \cdot (-1)^{|M|} \cdot \prod_{v \in V} (n + 2d(v) - 4)^{\overline{-|M_v|}}.$$

Taking expectations⁴ using Lemma 32, we expand $\mathbb{E}[m_{\text{route}_G(M)} \cdot m_H]$ into a sum over all completions C of the partial matching M (on the graph $G \cup H$). As in the Gaussian case, we collect terms based on the overall matching $M \cup C \in \mathcal{PM}(G \cup H)$. Performing the grouping of terms, we have

$$\begin{aligned} \mathbb{E} p_G m_H &= \sum_{M \in \mathcal{PM}(G \cup H)} n^{\text{cycles}_{G \cup H}(M)} \sum_{S \subseteq G\text{-pairs}} (-1)^{|S|} \cdot \prod_{v \in V} (n + 2d(v) - 4)^{\overline{-|S_v|}} \cdot n^{\overline{-d(v) + |S_v|}} \\ &= \sum_{M \in \mathcal{PM}(G \cup H)} n^{\text{cycles}(M)} \prod_{v \in V} \sum_{S_v \subseteq G\text{-pairs at } v} (-1)^{|S_v|} (n + 2d(v) - 4)^{\overline{-|S_v|}} \cdot n^{\overline{-d(v) + |S_v|}} \\ &= \sum_{M \in \mathcal{PM}(G \cup H)} n^{\text{cycles}(M)} \prod_{v \in V} \sum_{k=0}^{g_M(v)} \binom{g_M(v)}{k} (-1)^k (n + 2d(v) - 4)^{\overline{-k}} \cdot n^{\overline{-d(v) + k}}. \end{aligned}$$

The inner summation (with v fixed) is

$$\begin{aligned} &\sum_{k=0}^{g_M(v)} \binom{g_M(v)}{k} (-1)^k (n + 2d(v) - 4)^{\overline{-k}} \cdot n^{\overline{-d(v) + k}} \\ &= n^{\overline{-d(v)}} \sum_{k=0}^{g_M(v)} \binom{g_M(v)}{k} (-1)^k (n + 2d(v) - 4)^{\overline{-k}} \cdot (n + 2d(v) - 2)^{\overline{k}} \\ &= \frac{n^{\overline{-d(v)}}}{(n + 2d(v) - 4)^{\overline{g_M(v)}}} \sum_{k=0}^{g_M(v)} \binom{g_M(v)}{k} (-1)^k (n + 2d(v) - 2g_M(v) - 2)^{\overline{g_M(v) - k}} \cdot (n + 2d(v) - 2)^{\overline{k}} \\ &= \frac{n^{\overline{-d(v)}}}{(n + 2d(v) - 4)^{\overline{g_M(v)}}} \sum_{k=0}^{g_M(v)} \binom{g_M(v)}{k} (n + 2d(v) - 2g_M(v) - 2)^{\overline{g_M(v) - k}} \cdot (-n - 2d(v) + 2)^{\overline{k}}. \end{aligned}$$

Using the umbral formula $(x + y)^{\overline{m}} = \sum_{k=0}^m \binom{m}{k} x^{\overline{k}} y^{\overline{m-k}}$ [12],

$$\begin{aligned} &= \frac{n^{\overline{-d(v)}}}{(n + 2d(v) - 4)^{\overline{g_M(v)}}} (-2g_M(v))^{\overline{g_M(v)}} \\ &= \frac{n^{\overline{-d(v)}}}{(n + 2d(v) - 4)^{\overline{g_M(v)}}} (-2)^{\overline{g_M(v)}}. \end{aligned}$$

⁴ We should not remove the self-loops in $\text{route}_G(M)$ which is permitted by Remark 33.

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► **Corollary 43.** For G such that $|E(G)| \leq o(\log n / \log \log n)$,

$$\mathbb{E}[p_G^2] = n^{-|E(G)|+o(1)}.$$

Proof. We have

$$\prod_{v \in V} n^{\overline{-d(v)}} = \prod_{v \in V} n^{-d(v)+o(1)} = n^{-2|E(G)|+o(1)}.$$

The magnitude of the coefficient c_M is $n^{\text{cycles}(M)-g_M}$. Since G has no self-loops, the maximum number of cycles for $M \in \mathcal{PM}(G \cup G)$ is $|E(G)|$, therefore M has the largest magnitude of n if and only if M pairs each edge with a parallel edge from the other copy of the graph. For these M , $c_M = n^{|E(G)|}$. There is at least one such M and possibly up to $|PM(G, H)|$. Under the size assumption on G , $|PM(G, H)| = n^{o(1)}$ and therefore non-dominant terms are negligible,

$$\mathbb{E}[p_G^2] = n^{-2|E(G)|+|E(G)|+o(1)} = n^{-|E(G)|+o(1)}. \quad \blacktriangleleft$$

Up to the normalization factor of $\prod_{v \in V} n^{\overline{-d(v)}}$, the inner product is bounded by the same formula from the Gaussian case.

► **Corollary 44.** Let G and H be two multigraphs such that $G \leftrightarrow H$ with degrees $d(v)$, and $|E(G)|, |E(H)| \leq o(\log n / \log \log n)$. Then

$$|\mathbb{E}[p_G \cdot p_H]| \leq \prod_{v \in V} n^{\overline{-d(v)}} \sum_{M \in \mathcal{PM}(G, H)} n^{\text{cycles}(M)+o(1)}.$$

Proof. From Lemma 42,

$$\begin{aligned} \mathbb{E}[p_G \cdot p_H] &= \prod_{v \in V} n^{\overline{-d(v)}} \sum_{M \in \mathcal{PM}(G \cup H)} c_M \\ &= \prod_{v \in V} n^{\overline{-d(v)}} \sum_{M \in \mathcal{PM}(G \cup H)} n^{\text{cycles}(M)} \prod_{v \in V} \frac{(-2)^{\overline{g_M(v)}}}{(n + 2d(v) - 4)^{\overline{g_M(v)}}}. \end{aligned}$$

If M has both a G -pair and an H -pair at v , observe how the magnitude of c_M changes if we re-match them into two (G, H) -pairs to get a new matching M' . $g_M(v)$ goes down by 1, $\text{cycles}(M)$ may increase by 1, decrease by 1, or stay the same. Therefore the magnitude of $c_{M'}$ is at least as large as c_M . Iterating this, the dominant terms are $M \in \mathcal{PM}(G, H)$, and the size assumption means they are dominant up to a $n^{o(1)}$ factor. \blacktriangleleft

There are often significantly more cancellations than the Gaussian case. We conjecture that the magnitude for planar graphs $G \cup H$ is given by the *simple* matchings $M \in \mathcal{PM}(G, H)$.

► **Definition 45.** For a multigraph G and $M \in \mathcal{PM}(G)$, we say that M is v -simple if v is visited at most once in each cycle induced by M . We say that M is simple if every cycle is simple.

► **Conjecture 46.** Let G and H be two loopless multigraphs such that $G \cup H$ is planar, and $|E(G)|, |E(H)| \leq o(\log n / \log \log n)$. Then

$$\mathbb{E}[p_G \cdot p_H] = \frac{1}{n^{|E(G)|+|E(H)|}} \cdot \left(\sum_{\text{simple } M \in \mathcal{PM}(G, H)} n^{\text{cycles}(M)} \right) \cdot (1 \pm o(1)).$$

If there are no simple $M \in \mathcal{PM}(G, H)$, then the expectation is zero.

4 Polynomial Basis for the Boolean Setting

Let $H_n = \{-1, +1\}^n$. Letting $d_u \in_{\mathbb{R}} H_n$, let $\text{Sym}_{\text{bool}}^V$ be the set of polynomials p in the d_u which are symmetric under simultaneous automorphism of the hypercube: for any $\pi \in \text{Aut}(H_n)$,

$$p(d_1, \dots, d_u, \dots) = p(\pi d_1, \dots, \pi d_u, \dots).$$

$\text{Aut}(H_n)$ is well-known to be the hyperoctahedral group.

► **Fact 47.** $\text{Aut}(H_n)$ consists of permutations of the coordinates $[n]$ and bitflips using any $z \in \{-1, +1\}^n$. Formally, $\text{Aut}(H_n)$ is a semidirect product of S_n and \mathbb{Z}_2^n .

We give a nice basis for such functions, showing formulas that mirror the general theme of routings and matchings in the underlying graph.

► **Definition 48** (Generalized inner product). For d_1, \dots, d_{2k} , let

$$\langle d_1, \dots, d_{2k} \rangle = \sum_{i=1}^n d_{1,i} \cdots d_{2k,i}.$$

This is also denoted by the variable $x_{1, \dots, 2k}$.

We say that a hypergraph is even if the size of every hyperedge is even. Let $\deg_G(v)$ be the number of edges of G containing v . Given an even hypergraph G on vertex set $[m]$, let

$$m_G = \prod_{\{e_1, \dots, e_{2k}\} \in E(G)} x_{e_1, \dots, e_{2k}}.$$

Note that edges are allowed to repeat.

The m_G are not linearly independent. A basis is:

► **Lemma 49.** The set of m_G such that: there is $\sigma : E(G) \rightarrow [n]$ such that for all vertices $u \in V$ and edges $e, f \ni u$, $\sigma(e) \neq \sigma(f)$, is a basis for $\text{Sym}_{\text{bool}}^V$.

Proof. Expand

$$m_G = \sum_{\sigma: E(G) \rightarrow [n]} \prod_{e = \{e_1, \dots, e_{2k}\} \in E(G)} d_{e_1, \sigma(e)} \cdots d_{e_{2k}, \sigma(e)}.$$

If there is no such σ , then every term above has a square term $d_{ij}^2 = 1$. Therefore m_G simplifies to a lower-degree polynomial, and it can be expressed in terms of other m_G .

If there is a σ for G , then m_G contains a multilinear monomial with “shape” G , which is linearly independent from other m_G . More formally, to show linear independence, suppose $\sum_G c_G m_G = 0$ for some c_G not all zero. Taking a nonzero graph G with maximum number of edges, precisely the coefficient c_G appears on multilinear monomials with “shape” G , such as the monomial for σ , which is a contradiction. ◀

► **Corollary 50.** The set of m_G such that G has at most n hyperedges is linearly independent.

► **Remark 51.** The hyperedges are sets, so they don’t contain repeats (and thus G has no self-loops). If we did have an edge e with a repeated vertex i in G , we could delete two copies of i from e without affecting m_G because we always have that $d_{ij}^2 = 1$.

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As before, we can run Gram-Schmidt to orthogonalize the m_G . We will generalize matching collections to the Boolean case and use them to express the resulting polynomials p_G . In the Boolean case it is also useful to express p_G and various calculations as a sum over certain functions $\sigma : E(G) \rightarrow [n]$.

► **Definition 52.** Let $\mathcal{M}_{\text{bool}}(G)$ be the set of partitions of $E(G)$.

► **Definition 53.** For $M \in \mathcal{M}_{\text{bool}}(G)$ define the routed hypergraph $\text{route}(M)$ by replacing each block B by a single hyperedge containing $v \in V$ which are incident to an odd number of edges in B .

Any block such that every $v \in V$ is incident to an even number of edges in B is called a “closed block”. Closed blocks are deleted from $\text{route}(M)$.

► **Definition 54.** For $M \in \mathcal{M}_{\text{bool}}(G)$ define the notation $\text{cycles}(M)$ to be the number of closed blocks of the partition.

► **Definition 55.** Let $\mathcal{PM}_{\text{bool}}(G)$ be the set of partitions of $E(G)$ such that every block is closed.

Denote the falling and rising factorial by

$$x^{\underline{k}} := x(x-1)\cdots(x-k+1), \quad x^{\overline{k}} := x(x+1)\cdots(x+k-1).$$

► **Lemma 56.**

$$\mathbb{E}[m_G] = \sum_{\substack{\sigma: E(G) \rightarrow [n] \\ \text{s.t. } \forall i, \sigma^{-1}(i) \text{ even}}} 1 = \sum_{M \in \mathcal{PM}_{\text{bool}}(G)} n^{\text{cycles}(M)}.$$

Proof. The first equality is obtained by expanding m_G into a sum of over all $\sigma : E(G) \rightarrow [n]$, then using linearity of expectation. The second equality is obtained by casing on which values of $\sigma(e)$ are equal, which induces a partition of $E(G)$. We have that σ contributes to the first sum if and only if all of the blocks of the induced partition are closed. Once the partition is fixed, there are $n^{\text{cycles}(M)}$ ways to choose distinct values for each cycle. ◀

For now we give only one definition of p_G . The definition in terms of matchings is more complicated and is included in the full version of the paper.

► **Definition 57** (Generic construction from Proposition 4).

$$p_G = \sum_{\substack{\sigma: E(G) \rightarrow [n] \\ \text{s.t. } \forall e, f \ni u, \sigma(e) \neq \sigma(f)}} \prod_{e = \{e_1, \dots, e_{2k}\} \in E(G)} d_{e_1, \sigma(e)} d_{e_2, \sigma(e)} \cdots d_{e_{2k}, \sigma(e)}.$$

► **Lemma 58** (Automorphism-invariance). $p_G \in \text{Sym}_{\text{bool}}^V$.

Proof. Neither of the two types of H_n symmetries changes p_G . Coordinate permutation doesn’t change p_G because σ doesn’t depend on the names of the coordinates. Bitflips don’t change p_G because every hyperedge is even (so flips cancel out). ◀

► **Corollary 59.** p_G equals the output of the degree-orthogonal Gram-Schmidt process on the m_G .

We can easily compute the inner product of p_G and p_H in the Boolean case. The idea is that p_G and p_H only contain terms where each vertex appears in each block at most once. When we multiply p_G and p_H together, these blocks may merge, giving us blocks where each vertex appears at most twice. If there is a block where a vertex appears only once, this block will have zero expected value, so the only terms which have nonzero expected value are the terms where in each block, each vertex either doesn't appear or appears twice, once from a G -edge and once from an H -edge. We now make this argument more precise.

► **Definition 60.** Let $\mathcal{PM}_{\text{bool}}(G, H)$ be the set of partitions of $E(G) \cup E(H)$ such that for each vertex and each block, the number of G -edges containing the vertex equals the number of H -edges.

We say that a partition $M \in \mathcal{PM}_{\text{bool}}(G, H)$ is simple if for each block, each vertex appears at most 2 times.

► **Lemma 61.**

$$\mathbb{E}[p_G p_H] = |\Sigma(G, H)| = \sum_{\text{simple } M \in \mathcal{PM}_{\text{bool}}(G, H)} n^{\text{cycles}(M)}$$

where $\Sigma(G, H)$ is the set of functions $\sigma : E(G \cup H) \rightarrow [n]$ such that

- (i) For $e, f \in E(G)$ such that $e \cap f \neq \emptyset$, $\sigma(e) \neq \sigma(f)$.
- (ii) For $e, f \in E(H)$ such that $e \cap f \neq \emptyset$, $\sigma(e) \neq \sigma(f)$.
- (iii) For all u, i , the size of $\{u \in e \in E(G \cup H) : \sigma(e) = i\}$ is even. Note that from conditions (i) and (ii) it must be size either 0 or 2.

Proof. The first equality follows from expanding p_G, p_H and using linearity of expectation. The second equality follows from looking at the partition induced by σ . The definition of $\Sigma(G, H)$ exactly checks that this partition is simple and in $\mathcal{PM}_{\text{bool}}(G, H)$. ◀

► **Corollary 62.** $n^{|E(G)|} \leq \mathbb{E}[p_G^2] \leq (2|E(G)|)^{2|E(G)|} n^{|E(G)|}$.

Proof. Each cycle in M requires at least two edges, and hence the maximum magnitude is bounded by $n^{|E(G)|}$. Furthermore, this can be achieved by matching each edge with its duplicate. The number of partitions of a k -element set is at most k^k , which proves the upper bound. ◀

The inner product formula implies that all inner products are non-negative, so the Boolean case does not exhibit the “negative inner product” abnormality of the spherical case with the K_5 example.

5 Inversion Formula for Approximate Orthogonality

Consider the problem of Fourier inversion: given parameters $\hat{f}(G)$ for different graphs G , find an orthogonally invariant function $f : (\mathbb{R}^n)^V \rightarrow \mathbb{R}$ such that

$$\langle f, p_G \rangle = \hat{f}(G).$$

If the p_G were completely orthogonal, then the function

$$f = \sum_G \hat{f}(G) \cdot \frac{p_G}{\mathbb{E} p_G^2}$$

is the unique f in the span of p_G for given G . In general, let Q be the square matrix indexed by graphs G with entries $Q[G, H] := \langle p_G, p_H \rangle$. Then f is given by

$$f = \sum_G \left(\sum_H Q^{-1}[G, H] \cdot \widehat{f}(H) \right) \cdot p_G$$

provided that Q is invertible.

Because of approximate orthogonality, Q is close to a diagonal matrix. Therefore Q^{-1} is also close to a diagonal matrix. Formally we show

► **Lemma 63.** *Suppose we are in either the Gaussian, spherical, or Boolean setting. Let finitely many nonzero $\widehat{f}(G) \in \mathbb{R}$ be given where G is a graph of the appropriate type for the setting, and assume that $|E(G)| = o(\frac{\log n}{\log \log n})$ for all given G . For sufficiently large n , there is a unique f satisfying $\langle f, p_G \rangle = \widehat{f}(G)$, and f equals*

$$f = \sum_H (\widehat{f}(H) + o(1) \cdot \max_{G \leftrightarrow H} |\widehat{f}(G)|) \cdot \frac{p_H}{\mathbb{E} p_H^2}.$$

Proof. Since the p_G are orthogonal if $G \not\leftrightarrow H$, the matrix Q is block diagonal with blocks defined by \leftrightarrow . The bound on the size of G implies that the dimension of each block is $n^{o(1)}$.

The diagonal terms are

$$\mathbb{E}[p_G^2] = \begin{cases} n^{|E(G)|+o(1)} & \text{Gaussian case (Corollary 25)} \\ n^{-|E(G)|+o(1)} & \text{Spherical case (Corollary 43)} \\ n^{|E(G)|+o(1)} & \text{Boolean case (Corollary 62)} \end{cases}$$

The off-diagonal terms with $G \leftrightarrow H$ are bounded by

$$|\mathbb{E}[p_G p_H]| \leq \begin{cases} \max_{M \in \mathcal{PM}(G, H)} n^{\text{cycles}(M)+o(1)} & \text{Gaussian case (Lemma 23)} \\ n^{-2|E(G)|} \max_{M \in \mathcal{PM}(G, H)} n^{\text{cycles}(M)+o(1)} & \text{Spherical case (Corollary 44)} \\ \max_{\text{simple } M \in \mathcal{PM}_{\text{bool}}(G, H)} n^{\text{cycles}(M)+o(1)} & \text{Boolean case (Lemma 61)} \end{cases}$$

When $G \neq H$, we claim that $\text{cycles}(M)$ must be strictly less than $|E(G)|$. Any $M \in \mathcal{PM}(G, H)$ achieving $|E(G)|$ cycles must pair up edges of G and H , which shows the contrapositive.

Therefore the off-diagonal terms are smaller by a factor of $n^{1-o(1)}$ than the diagonal term. Therefore Q is invertible (for sufficiently large n) and

$$Q^{-1}[G, H] = \begin{cases} \frac{1}{\mathbb{E}[p_G^2]} & G = H \\ n^{o(1)-1} \cdot \frac{1}{\mathbb{E}[p_G^2]} & G \neq H \end{cases} \quad \blacktriangleleft$$

► **Remark 64.** Using more careful counting, the assumption on $|E(G)|$ can likely be improved to $|E(G)| \leq n^\delta$ for some explicit $\delta > 0$.

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