Unified Statistical Theory of Spectral Graph Analysis

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Dedicated to the beloved memory of Emanuel (Manny) Parzen.

Abstract

The goal of this paper is to show that there exists a simple, yet universal\(^1\) statistical logic of spectral graph analysis by recasting it into a nonparametric function estimation problem. The prescribed viewpoint appears to be good enough to accommodate most of the existing spectral graph techniques as a consequence of just one single formalism and algorithm.

Keywords and phrases: Nonparametric spectral graph analysis; Graph correlation density field (GraField); Empirical and smoothed spectral graph analysis; High-dimensional discrete data smoothing.

Contents

1 Introduction
1.1 Spectral Graph Analysis: A Practitioner’s Guide
1.2 Previous Theoretical Treatments
1.3 A Set of Questions
1.4 Unified Construction Principle

2 Fundamentals of Statistical Spectral Graph Analysis
2.1 Graph Correlation Density Field
2.2 Karhunen-Loève Representation of Graph
2.3 Nonparametric Spectral Approximation Theory

3 Empirical Spectral Graph Analysis
3.1 Laplacian Spectral Analysis
3.2 Diffusion Map
3.3 Modularity Spectral Analysis

4 Smoothed Spectral Graph Analysis
4.1 High-dimensional Undersampled Regime
4.2 Spectral Smoothing
4.3 Type-I Regularized Graph Laplacian
4.4 Type-II Regularized Graph Laplacian
4.5 Google’s PageRank Method
4.6 Other Generalizations

5 Application to Graph Regression

6 Concluding Remarks

\(^1\)By universal, I mean the theory should not be specific to any particular spectral graph analysis technique but be meaningfully applicable to a class of models.
1 Introduction

Spectral graph data analysis is undoubtedly the most favored technique for graph data analysis, both in theory and practice. It has been extraordinarily successful in many applications including data mining, web search, quantum computing, computer vision, image segmentation, and others. Over the last several decades, extensive efforts have been made by researchers and practitioners to develop a suite of spectral graph analysis techniques (e.g., Laplacian, Modularity, Diffusion map, regularized Laplacian, Google PageRank model etc.) with increasing sophistication and specialization. However, no single algorithm can be regarded as a panacea for dealing with the evolving complexities of modern graphs. Therefore, the most important and pressing question for the field today appears to be whether we can develop a unifying language to establish “bridges” between a wide variety of spectral graph analysis techniques, and thus providing logically connected means for reaching different ends. Undoubtedly, any such formulation would be of great theoretical significance and practical value, that will ultimately provide the applied data scientists clear guidance and a systematic strategy for selecting the proper spectral tools to arrive at a confident conclusion.

To that end, this work attempts to unify the theories of spectral graph analysis by purely statistical means. That is, we seek a constructive (rather than confirmatory) theoretical framework integrating classical and modern spectral graph analysis algorithms, which to date have been viewed as distinct methods.

1.1 Spectral Graph Analysis: A Practitioner’s Guide

The way spectral graph analysis is currently taught and practiced can be summarized as follows (also known as spectral heuristics):

1. Let \( G = (V, E) \) denotes a (possibly weighted) undirected graph with a finite set of vertices \(|V| = n\), and a set of edges \( E \). Represent the graph using weighted adjacency matrix \( A \) where \( A(x, y; G) = w_{xy} \) if the nodes \( x \) and \( y \) are connected by an edge and 0 otherwise; weights are non-negative and symmetric.

2. Define “suitable” spectral graph matrix (also known as graph “shift” operator). Most popular and successful ones are listed below:

\[
\begin{align*}
\mathcal{L} &= D^{-1/2} AD^{-1/2}; \quad \text{Chung}\ (1997) \\
\mathcal{B} &= A - N^{-1}dd^T; \quad \text{Newman}\ (2006) \\
\mathcal{T} &= D^{-1}A; \quad \text{Coifman and Lafon}\ (2006) \\
\text{Type-I Reg. } \mathcal{L}_\tau &= D^{-1/2} A D^{-1/2}; \quad \text{Chaudhuri et al.}\ (2012) \\
\text{Type-II Reg. } \mathcal{L}_\tau &= D^{-1/2} A \tau D^{-1/2}; \quad \text{Amini et al.}\ (2013) \\
\text{Google’s PageRank } \mathcal{T}_\alpha &= \alpha D^{-1}A + (1 - \alpha)F; \quad \text{(Brin and Page}\ 1999) \\
\end{align*}
\]

\( D = \text{diag}(d_1, \ldots, d_n) \in \mathbb{R}^{n \times n} \), \( d_i \) denotes the degree of a node, \( \tau > 0 \) regularization parameter, \( F \in \mathbb{R}^{n \times n} \) with all entries \( 1/n \), and \( N = 2|E| = \sum_{x,y} A(x, y) \).
3. Perform spectral decomposition of the matrix selected at step 2, whose eigenvectors form an orthogonal basis of $\mathbb{R}^n$. Spectral graph theory seeks to understand the interesting properties and structure of a graph by using leading nontrivial eigenvectors and eigenvalues, first recognized by Fiedler (1973), which provide the basis for performing harmonic analysis on graphs.

4. Compute graph Fourier transform (GFT) by expanding functions (or signals) defined over the vertices of a graph as a linear combination of the selected eigenbasis (from step 3) and carry out learning tasks such as regression, clustering, classification, smoothing, kriging, etc.

1.2 Previous Theoretical Treatments

There has been a flood of publications on statistical spectral graph theory, most of which have focused on asymptotic justifications of different techniques (mentioned in the previous section). See, in particular, those based on Laplacian (Von Luxburg et al., 2008, Belkin and Niyogi, 2001), modularity (Davis and Sethuraman, 2016), diffusion map (Coifman and Lafon, 2006, Coifman et al., 2005), and regularized Laplacian (Chaudhuri et al., 2012, Le et al., 2015) methods. More refined theoretical results in the context of a specific parametric graph model (such as stochastic block model or its variants) are discussed in Joseph and Yu (2016), Rohe et al. (2011), Sarkar et al. (2015) and Qin and Rohe (2013).

What is this paper not about? It is important to draw a distinction between the theory that purports to provide the constructions of different spectral graph techniques and, the theory that does not. This article focuses on the former. Instead of statistical confirmation, here our main interest lies in understanding the statistical origins of various spectral graph techniques. This is mostly ill-understood and neglected territory. The current theoretical treatments do not give us any clues on this issue.

1.3 A Set of Questions

Despite many advances, the theory and practice of spectral graph analysis are still very much compartmentalized and unsystematic. The graph signal processing engineers are often left bewildered by the vastness of the existing literature and huge diversity of methods (developed by the machine learning community, applied harmonic analysts, physicists, and statisticians). This has led to a need to develop a broader perspective on this topic, lest we be guilty of not seeing the forest for the trees. The question how different spectral graph techniques can naturally originate from some underlying basic principle, plays the key role in this regard by clarifying the mystery of why and when to use them. The reality is we still lack general tools and techniques to attack this question in a statistical way. Given the very different character of the existing spectral models, it seems that new kinds of abstractions need to be formulated to address this fundamental challenge. What would these abstractions look like? How can we discover a statistical path that naturally leads to these different spectral methods? One such promising theory is discussed in this paper,
taking inspiration from celebrated history on nonparametric spectral analysis of time series. The prescribed modern viewpoint shows an exciting confluence of nonparametric function estimation, quantile domain methods, and Fourier harmonic analysis to unveil a more simple conceptual structure of this subject, avoiding undue complexities.

1.4 Unified Construction Principle

We start by giving a glance to the unified spectral representation scheme, whose (nonparametric) statistical interpretation and justification is deferred until the next section, as it requires a more technical background. It turns out that all known spectral graph techniques are just different manifestations of this single general algorithm in some way.

Probability Notations and Definitions. We will stick to the following probabilistic notations. Define network probability mass function by

\[ P(x, y; G) = \frac{A(x, y; G)}{\sum x, y A(x, y; G)}; \]

Vertex probability mass function by

\[ p(x; G) = \sum y P(x, y; G) \]

and

\[ p(y; G) = \sum x P(x, y; G). \]

Finally, define the important Graph Interaction Function by

\[ GIF(x, y; G) = \frac{P(x, y; G)}{p(x; G)p(y; G)}, \]

where \( x, y \in V(G) \).

Algorithm 1. Nonparametric Spectral Graph Analysis: A Unified Algorithm

**Step 1.** For given discrete graph \( G \) of size \( n \), construct GraField kernel function \( C : [0, 1]^2 \to \mathbb{R}_+ \cup \{0\} \) defined a.e by

\[ C(u, v; G) = GIF[Q(u; X), Q(v; Y); G] = \frac{P(Q(u; X), Q(v; Y); G)}{p(Q(u; X))p(Q(v; Y))}, \]

where \( u = F(x; G) \), \( v = F(y; G) \) for \( x, y \in \{1, 2, \ldots, n\} \).

**Step 2.** Let \( \{\xi_j\}_{j \geq 0} \) be a complete orthonormal system on \([0, 1]\). Construct discrete transform basis \( \xi_j(x; F(X; G)) := \xi_j(F(x; G)) \), evaluated at the vertex-rank-transforms. They satisfy the following orthonormality conditions (degree-weighted):

\[ \sum_x \xi_j(x; F(X)) \xi_k(x; F(X)) p(x; G) = \delta_{jk}, \]

thus constitutes an orthonormal basis for \( L^2(F; G) \).

**Step 3.** Transform coding of graphs. Construct generalized spectral graph matrix \( M(G, \xi) \in \mathbb{R}^{n \times n} \) with respect to \( \eta_j(u) := \xi_j(Q(u; X); F) \):

\[ M[j, k; G, \xi] = \left\langle \eta_j, \int_0^1 (C - 1) \eta_k \right\rangle_{L^2[0, 1]} = \sum_{\ell, m} \xi_j(\ell; F) \xi_k(m; F) P(\ell, m; G). \]

\( M_\xi \) can be viewed as a transform coefficient matrix of the orthogonal series expansion of \( C(u, v; G) \) with respect to the product bases \( \{\eta_j \eta_k\}_{1 \leq j, k \leq n} \).
Step 4. Perform the singular value decomposition (SVD) of $M_\xi = U\Lambda U^T = \sum_k u_k \mu_k u_k^T$, where $u_{ij}$ are the elements of the singular vector of moment matrix $U = (u_1, \ldots, u_n)$, and $\Lambda = \text{diag}(\mu_1, \ldots, \mu_n), \mu_1 \geq \cdots \geq \mu_n \geq 0$.

Step 5. Obtain approximate Karhunen-Loéve (KL) representation basis (which acts as a graph Fourier basis) of the graph $\mathcal{G}$ by

$$\tilde{\phi}_k = \sum_{j=1}^{n} u_{jk} \xi_j, \text{ for } k = 1, \ldots, n - 1,$$

which can be directly used for subsequent signal processing on graphs.

Organization. The next section is devoted to the fundamental principles that underlie this algorithm. The unifying power will be shown in Sections 3 and 4. By doing so, we will introduce empirical and smooth spectral graph analysis techniques. We also address the open problem of obtaining a formal interpretation of “spectral regularization”. A deep connection between high-dimensional discrete data smoothing and spectral regularization is discovered. This new perspective provides, for the first time, the theoretical motivation and fundamental justification for using regularized spectral methods, which were previously considered to be empirical guesswork-based ad hoc solutions. Important application towards spatial graph regression is discussed in Section 5. In Section 6, we end with concluding remarks. Additional applications are available as supplementary materials.

2 Fundamentals of Statistical Spectral Graph Analysis

2.1 Graph Correlation Density Field

Wiener’s generalized harmonic analysis formulation on spectral representation theory of time series starts by defining the autocorrelation function (ACF) of a signal. In particular, Wiener–Khintchine theorem asserts ACF and the spectral density are Fourier duals of each other. Analogous to Wiener’s correlation technique, we describe a new promising starting point, from which we can develop the whole spectral graph theory systematically by bringing nonparametric function estimation and harmonic analysis perspectives. Both statistical and probabilistic motivations will be given.

Definition 1. For given discrete graph $\mathcal{G}$ of size $n$, the piecewise-constant bivariate kernel function $\mathcal{C} : [0,1]^2 \to \mathbb{R}_+ \cup \{0\}$ is defined almost everywhere through

$$\mathcal{C}(u,v;\mathcal{G}_n) = \text{GIF}[Q(u;X),Q(v;Y);\mathcal{G}_n] = \frac{p(Q(u;X),Q(v;Y);\mathcal{G}_n)}{p(Q(u;X))p(Q(v;Y))}, \quad 0 < u, v < 1. \quad (2.1)$$

Theorem 1. GraField defined in Eq. (2.1) is a positive piecewise-constant kernel satisfying

$$\iint_{[0,1]^2} \mathcal{C}(u,v;\mathcal{G}_n) \, du \, dv = \sum_{(i,j) \in \{1,\ldots,n\}^2} \iint_{I_{ij}} \mathcal{C}(u,v;\mathcal{G}_n) \, du \, dv = 1,$$
where
\[ I_{ij}(u,v) = \begin{cases} 1, & \text{if } (u,v) \in (F(i;X), F(i+1;X)) \times (F(j;Y), F(j+1;Y))] \\ 0, & \text{elsewhere} \end{cases} \]

**Note 1.** The bivariate step-like shape of the GraField kernel is governed by the (piecewise-constant left continuous) quantile functions \( Q(u;X,G_n) \) and \( Q(v;Y,G_n) \) of the discrete vertex probability measures. As a result, in the continuum limit (let \( (G_n)_{n \geq 0} \) be a sequence of graphs whose number of vertices tends to infinity \( n \to \infty \)), the shape of the piecewise-constant discrete \( C_n \) approaches a “continuous field” over unit interval – a self-adjoint compact operator on square integrable functions (defined on the graph) with respect to vertex probability measure \( p(x;G) \) (see Section 2.2 for more details).

**Motivation 1.** We start with a diffusion based probabilistic interpretation of the GraField kernel. The crucial point to note is that the “slices” of the \( C \) (2.1) can be expressed as \( p(y|x;G)/p(y;G) \) in the vertex domain. This alternative conditional probability-based viewpoint suggests a connection with the random walk on the graph. Interpret \( p(y|x;G) \) as transition probability from vertex \( x \) to vertex \( y \) in one time step. Also note that \( p(y;G) \) is the stationary probability distribution on the graph, as we have \( \lim_{t \to \infty} p(t,y|x;G) = p(y;G) \) regardless of the initial starting point \( x \) (moreover, for connected graphs the stationary distribution is unique). Here \( p(t,y|x;G) \) denotes the probability distribution of a random walk landing at location \( y \) at time \( t \), starting at the vertex \( x \). See Lovász (1993) for an excellent survey on the theory of random walks on graphs.

The graph affinity function measures how the transition probability \( p(y|x;G) \) is different from the “baseline” stationary distribution (long-run stable behavior) \( p(y;G) \). That comparison ratio is the fundamental interaction function for graphs which we denote by \( \text{GIF}(x,y;G) \). This probabilistic interpretation along with Theorem 2 and 5 will allow us to integrate the diffusion map (Coifman and Lafon, 2006) technique into our general statistical framework in Section 3.2.

**Motivation 2.** GraField compactly represents the affinity or strength of ties (or interactions) between every pair of vertices in the graph. To make this clear, let us consider the following adjacency matrix of a social network representing 4 employees of an organization

\[
A = \begin{pmatrix}
0 & 2 & 0 & 0 \\
2 & 0 & 3 & 3 \\
0 & 3 & 0 & 3 \\
0 & 3 & 3 & 0
\end{pmatrix},
\]

where the weights reflect numbers of communication (say email messages or coappearances in social events etc.). Our interest lies in understanding the strength of association between the employees i.e., \( \text{Strength}(x,y) \) for all pairs of vertices. Looking at the matrix \( A \) (or equivalently based on the histogram network estimator \( p(x,y;G) = A/N \) with \( N = \sum_{x,y} A(x,y) = 22 \)) one might be tempted to conclude that the link between
employee 1 and 2 is the weakest, as they have communicated only twice, whereas employees 2, 3, and 4 constitute strong ties, as they have interacted more frequently. Now, the surprising fact is that (i) Strength(1, 2) is twice that of Strength(2, 3) and Strength(2, 4); also (ii) Strength(1, 2) is 1.5 times of Strength(3, 4)!

To understand this paradox, compute the vertex-domain empirical GraField kernel matrix (Definition 1) with \((x, y)\)th entry
\[ N \cdot A(x, y; \mathcal{G})/d(x)d(y) \]

\[
\mathcal{C}_n = \begin{pmatrix}
0 & 22/8 & 0 & 0 \\
22/8 & 0 & 22/16 & 22/16 \\
0 & 22/16 & 0 & 22/12 \\
0 & 22/16 & 22/12 & 0
\end{pmatrix}.
\]

This toy example is in fact a small portion (with members 1, 9, 31 and 33) of the famous Zachary’s karate club data, where the first two members were from Mr. Hi’s group and the remaining two were from John’s group. The purpose of this illustrative example is not to completely dismiss the adjacency or empirical graphon (Lovász and Szegedy, 2006) based analysis but to caution the practitioners so as not to confuse the terminology “strength of association” with “weights” of the adjacency matrix – the two are very different objects. Existing literature uses them interchangeably without paying much attention. The crux of the matter is: association does not depend on the raw edge-density, it is a “comparison edge-density” that is captured by the GraField; see Section 3.2 for its intriguing connection with diffusion based graph-distance.

**Motivation 3.** GraField can also be viewed as properly “renormalized Graphon,” which is reminiscent of Wassily Hoeffding’s “standardized distributions” idea (Hoeffding, 1940). Thus, it can be interpreted as a discrete analogue of copula (the Latin word copula means “a link, tie, bond”) density for random graphs that captures the underlying correlation field. We study the structure of graphs in the spectral domain via this fundamental graph kernel \(\mathcal{C}\) that characterizes the implicit connectedness or tie-strength between pairs of vertices.

Fourier-type spectral expansion results of the density matrix \(\mathcal{C}\) are discussed in the ensuing section, which is at the heart of our approach. We will demonstrate that this correlation density operator-based formalism provides a useful perspective for spectral analysis of graphs that allows unification.

### 2.2 Karhunen-Loéve Representation of Graph

We define the Karhunen-Loéve (KL) representation of a graph \(\mathcal{G}\) based on the spectral expansion of its GraField function \(\mathcal{C}(u, v; \mathcal{G})\). Schmidt decomposition (Schmidt, 1907) of \(\mathcal{C}\) yields the following spectral representation theorem of the graph.

**Theorem 2.** The square integrable graph correlation density kernel \(\mathcal{C} : [0, 1]^2 \to \mathbb{R}_+ \cup \{0\}\) of two-variables admits the following canonical representation

\[
\mathcal{C}(u, v; \mathcal{G}_n) = 1 + \sum_{k=1}^{n-1} \lambda_k \phi_k(u)\phi_k(v),
\]
where the non-negative $\lambda_1 \geq \lambda_2 \geq \cdots \lambda_{n-1} \geq 0$ are singular values and $\{\phi_k\}_{k \geq 1}$ are the orthonormal singular functions $\langle \phi_j, \phi_k \rangle_{\mathcal{L}^2[0,1]} = \delta_{jk}$, for $j, k = 1, \ldots, n - 1$, which can be evaluated as the solution of the following integral equation relation

$$
\int_{[0,1]} [\mathcal{C}(u,v; \mathcal{G}) - 1] \phi_k(v) \, dv = \lambda_k \phi_k(u), \quad k = 1, 2, \ldots, n - 1.
$$

(2.3)

**Remark 1.** By virtue of the properties of Karhunen-Loéve (KL) expansion [Loève 1955], the eigenfunction basis $\phi_k$ satisfying [2.3] provides the optimal low-rank representation of a graph in the mean square error sense. In other words, $\{\phi_k\}$ bases capture the graph topology in the smallest embedding dimension and thus carries practical significance for graph compression. Hence, we can call those functions the *optimal* coordinate functions or Fourier representation bases. Accordingly, the fundamental statistical modeling problem hinges on finding approximate solutions to the optimal graph coordinate system $\{\phi_1, \ldots, \phi_{n-1}\}$ satisfying the integral equation [2.3].

**Definition 2.** Any function or signal $y \in \mathbb{R}^n$ defined on the vertices of the graph $y : V \mapsto \mathbb{R}$ such that $\|y\|^2 = \sum_{x \in V(\mathcal{G})} |y(x)|^2 p(x; \mathcal{G}) < \infty$, can be represented as a linear combination of the Schmidt bases of the GraField density matrix $\mathcal{C}$. Define the *generalized graph Fourier transform* of $y$

$$
\hat{y}(\lambda_k) := \langle y, \phi_k \rangle = \sum_{x=1}^n y(x) \phi_k[F(x; \mathcal{G})].
$$

This spectral or frequency domain representation of a signal, belonging to the square integrable Hilbert space $\mathcal{L}^2(F; \mathcal{G})$ equipped with the inner product

$$
\langle y, z \rangle_{\mathcal{L}^2(F, \mathcal{G})} = \sum_{x \in V(\mathcal{G})} y(x) z(x) p(x; \mathcal{G}),
$$

allows us to construct efficient graph learning algorithms. As $\{\phi_k\}$’s are KL spectral bases, the vector of projections onto this basis function decay rapidly, and hence may be truncated aggressively to capture the structure in a small number of bits.

**Definition 3.** The entropy (or energy) of a discrete graph $\mathcal{G}$, is defined using the Parseval relation of the canonical representation

$$
\text{Entropy}(\mathcal{G}) = \int_{[0,1]^2} (\mathcal{C} - 1)^2 \, du \, dv = \sum_k |\lambda_k|^2.
$$

This quantity, which captures the departure of uniformity of the $\mathcal{C}$, can be interpreted as a measure of ‘structure’ or the ‘compressibility’ of the graph. Entropy measure can also be used to (i) define graph homogeneity and (ii) design fast algorithms for graph isomorphism. For homogeneous graphs, the shape of the correlation density field is uniform over the unit square. The power at each harmonic components, as a function of frequency, is called the power spectrum of the graph. Flat spectrum is equivalent to the analogous notion of white-noise process.

8
2.3 Nonparametric Spectral Approximation Theory

We view the spectral graph learning algorithm as a method of approximating \((\lambda_k, \phi_k)_{k \geq 1}\) that satisfies the integral equation (2.3), corresponding to the graph kernel \(C(u, v; G)\). In practice, often the most important features of a graph can be well characterized and approximated by a few top (dominating) singular-pairs. The statistical estimation problem can be summarized as follows:

\[
A_{n \times n} \mapsto C \mapsto \{(\hat{\lambda}_1, \hat{\phi}_1), \ldots, (\hat{\lambda}_{n-1}, \hat{\phi}_{n-1})\} \text{ that satisfies Eq. (2.3).}
\]

2.3.1 From Continuous to Discrete Basis and Back

The Fourier-type nonparametric spectral approximation method starts by choosing an expansion basis. Let \(\xi_j\) denote an orthonormal basis of \(L^2[0, 1]\). Construct the discrete transform basis of \(\mathbb{R}^n\) by evaluating \(\xi_j\) at the vertex-rank-transforms \(\xi_j(F(x; G)) := \xi_j(x; F, G)\). Verify that \(\xi_j(x; F, G)\) are orthogonal with respect to the measure \(p(x; G)\) satisfying

\[
\sum_x \xi_j(x; F, G) \xi_j(x; F, G) p(x; G) = 0, \text{ for } j \neq k.
\]

Thus form an orthogonal basis of the Hilbert space \(L^2(F; G)\). Define \(\eta\)-functions (quantile domain unit bases), generated from mother \(\xi_j\) by

\[
\eta_j(u; G) = \xi_j[Q(u; X); F, G], \quad 0 < u < 1,
\]

as piecewise-constant (left-continuous) functions over the irregular grid \(\{0, p(1), p(1) + p(2), \ldots, \sum_{j=1}^n p(j) = 1\}\) satisfying \(\langle \eta_j, \eta_k \rangle_{L^2[0,1]} = 0\), if \(j \neq k\). They will provide a useful tool to recast conventional matrix calculus-based approaches as a functional statistical problem. One unique aspect of our construction is that in the continuum limit (as the size of the graph \(n \to \infty\)) the discrete \(\eta\)-basis of \(\mathbb{R}^n\) approaches the mother \(\xi\)-function, a basis of \(L^2[0, 1]\). We call it asymptotic “reproducing” property.

2.3.2 Projection Methods for Eigenvector Approximation

We are interested in the nonparametric estimation of eigenpairs \((\lambda_k, \phi_k)_{k \geq 0}\). Approximate the unknown eigenvectors by the projection, \(P_n \phi_k\), on the \(\text{span}\{\eta_j, j = 1, \ldots, n\}\) defined by

\[
\phi_k(u) \approx P_n \phi_k = \sum_{j=1}^n \theta_{jk} \eta_j(u), \quad 0 < u < 1 \tag{2.4}
\]

where \(\theta_{jk}\) are the unknown coefficients to be estimated.

**Definition 4** (Orthogonal Discrete Graph Transform). We introduce a generalized concept of matrices associated with graphs called the \(G\)-matrix. Define discrete graph transform with respect to an orthonormal system \(\eta\) as

\[
\mathcal{M}[j, k; \eta, G] = \left\langle \eta_j, \frac{1}{0} (\mathcal{G} - 1) \eta_k \right\rangle_{L^2[0,1]} \quad \text{for } j, k = 1, \ldots, n. \tag{2.5}
\]
Equivalently, we can define the discrete graph transform to be the coefficient matrix of the orthogonal series expansion of the GraField kernel $\mathcal{C}(u,v;G)$ with respect to the product bases \{\eta_j \eta_k\}_{1 \leq j,k \leq n}. As a practical significance, this generalization provides a systematic recipe for converting the graph problem into a “suitable” matrix problem:

$$
\mathcal{G}_n(V,E) \rightarrow A_{n \times n} \rightarrow \mathcal{C}(u,v;\mathcal{G}_n) \xrightarrow{\{\eta_1,\ldots,\eta_n\}} \mathcal{M}(\eta,G) \in \mathbb{R}^{n \times n}.
$$

**Theorem 3.** The $G$-matrix (2.5) can also be interpreted as a “covariance” operator for a discrete graph by recognizing the following equivalent representation for $x,y \in \{1,2,\ldots,n\}$

$$
\mathcal{M}[j,k;\xi,G] = \mathbb{E}_{P} \left[ \xi_j(F(X;G)) \xi_k(F(Y;G)) \right] = \sum_{x,y} P(x,y;G) \xi_j(F(x;G)) \xi_j(F(y;G)),
$$

This can be proved using the basic quantile mechanics fact that $Q(F(X)) = X$ holds with probability 1 (see Parzen (1979)). Next, we present a general approximation scheme that provides an effective method of discrete graph analysis in the frequency domain.

**Theorem 4** (Nonparametric spectral approximation). The Fourier coefficients \{\theta_{jk}\} of the projection estimators (2.4) of the GraField eigenfunctions (eigenvalues and eigenvectors), satisfying the integral equation (2.3), can be obtained by solving the following generalized matrix eigenvalue problem

$$
\mathcal{M} \Theta = S \Theta \Delta, \quad (2.6)
$$

where $\mathcal{M}_{jk} = \langle \eta_j, \int_0^1 (\mathcal{C}_n - 1) \eta_k \rangle_{L^2[0,1]}$, and $S_{jk} = \langle \eta_j, \eta_j \rangle_{L^2[0,1]}$.

To prove define the residual of the governing equation (2.3) by expanding $\phi_k$ as series expansion (2.4),

$$
R(u) \equiv \sum_j \theta_{jk} \left[ \int_0^1 (\mathcal{C}(u,v;G) - 1) \eta_j(v) dv - \lambda_k \eta_j(u) \right] = 0. \quad (2.7)
$$

Now for complete and orthonormal \{\eta_j\} requiring the error $R(u)$ to be zero is equivalent to the statement that $R(u)$ is orthogonal to each of the basis functions

$$
\langle R(u), \eta_k(u) \rangle_{L^2[0,1]} = 0, \quad k = 1,\ldots,n. \quad (2.8)
$$

This leads to the following set of equations:

$$
\sum_j \theta_{jk} \left[ \int_{[0,1]^2} (\mathcal{C}(u,v;G_n) - 1) \eta_j(v) \eta_k(u) dv du \right] - \lambda_k \sum_j \theta_{jk} \left[ \int_0^1 \eta_j(u) \eta_k(u) du \right] = 0. \quad (2.9)
$$

Theorem 4 plays a key role in our statistical reformulation. In particular, we will show how the fundamental equation (2.6) provides the desired unity among different spectral graph techniques by systematically constructing a “suitable” class of coordinate functions.
Note 2. The fundamental idea behind the Rietz-Galerkin style approximation scheme for solving variational problems in Hilbert space played a pivotal inspiring role to formalize the statistical basis of the proposed computational approach.

Note 3. Our nonparametric spectral approximation theory based on eigenanalysis of $G$-Matrix, remains unchanged for any choice $\eta$-function (following the recipe for construction given in Sec 2.3.1), which paves the way for the generalized harmonic analysis of graphs.

The next two sections investigate this general scheme under various choices of $\eta$-functions, and nonparametric estimation methods of $\mathcal{C}_n$. By doing so, many “mysterious similarities” among different spectral graph algorithms are discovered which were not known before.

3 Empirical Spectral Graph Analysis

Three popular traditional spectral graph analysis models will be synthesized in this section.

3.1 Laplacian Spectral Analysis

Laplacian is probably the most heavily used spectral graph technique in practice. Here we will demonstrate for the first time how the Laplacian of a graph naturally originates by purely statistical reasoning, totally free from the classical combinatorial based logic.

Degree-Adaptive Block-pulse Basis Functions. One of the fundamental, yet universally valid (for any graph) choice for $\{\eta_j\}_{1 \leq j \leq n}$ is the indicator top hat functions (also known as block-pulse basis functions, or in short BPFs). However, instead of defining the BPFs on a uniform grid (which is the usual practice) here (following Sec 2.3.1) we define them on the non-uniform mesh $0 = u_0 < u_1 \cdots < u_n = 1$ over $[0,1]$, where $u_j = \sum_{x \leq j} p(x; X)$ with local support

$$
\eta_j(u) = \begin{cases} 
    p^{-1/2}(j) & \text{for } u_{j-1} < u \leq u_j; \\
    0 & \text{elsewhere.}
\end{cases}
$$

(3.1)

They are disjoint, orthogonal, and a complete set of functions satisfying

$$
\int_0^1 \eta_j(u) \, du = \sqrt{p(j)}, \quad \int_0^1 \eta_j^2(u) \, du = 1, \quad \text{and} \quad \int_0^1 \eta_j(u) \eta_k(u) \, du = \delta_{jk}.
$$

Note 4. The shape (amplitudes and block lengths) of our specially designed BPFs depend on the specific graph structure via $p(x; \mathcal{G})$ as shown in Fig 1. In order to obtain the spectral domain representation of the graph, it is required to estimate the spectra of GraField kernel $\phi_k$, by representing them as block pulse series. The next result describes the required computational scheme for estimating the unknown expansion coefficients $\{\theta_{jk}\}$.

Theorem 5. Let $\phi_1, \ldots, \phi_n$ the canonical Schmidt bases of $L^2$ graph kernel $\mathcal{C}(u, v; \mathcal{G})$, satisfying the integral equation (2.3). Then the empirical solution of (2.3) for block-pulse
Figure 1: Two graphs and their corresponding degree-adaptive block-pulse functions. The amplitudes and the block length of the indicator basis functions \(3.1\) depends on the degree distribution of that graph.

Orthogonal series approximated \(3.1\) Fourier coefficients \(\{\theta_{jk}\}\) can equivalently be written down in closed form as the following matrix eigen-value problem

\[
\mathcal{L}^*[\theta] = \lambda\theta, \tag{3.2}
\]

where \(\mathcal{L}^* = \mathcal{L} - uu^T\), \(\mathcal{L}\) is the Laplacian matrix, \(u = D_p^{1/2}1_n\), and \(D_p = \text{diag}(p_1, \ldots, p_n)\).

Note that the discrete GraField kernel takes value \(\text{GIF}(j, k; G_n) = P(j, k; G_n)/p(j; G_n)p(k; G_n)\) and the tensor–product bases \(\eta_j(u)\eta_k(v)\) take value \(p^{-1/2}(j; G_n)p^{-1/2}(k; G_n)\) over the rectangle \(I_{jk}(u,v)\) for \(0 < u, v < 1\). This observation reduces the master equation \(2.9\) to the following system of linear algebraic equations expressed in the vertex domain:

\[
\sum_j \theta_{jk} \left[ \frac{p(j, k)}{\sqrt{p(j)p(k)}} - \sqrt{p(j)}\sqrt{p(k)} - \lambda_k\delta_{jk} \right] = 0. \tag{3.3}
\]
Empirical plugin nonparametric estimator. The estimating equation (3.3) contains unknown network and vertex probability mass functions which need to be estimated from the data. The most basic nonparametric estimates are \( \tilde{\mathcal{P}}(j,k;\mathcal{G}_n) = \frac{A[j,k;\mathcal{G}_n]}{N} \) and \( \tilde{p}(j;\mathcal{G}_n) = \frac{d(j;\mathcal{G}_n)}{N} \). By plugging these empirical estimators into Eq. (3.3), said equation can be rewritten as the following compact matrix form:

\[
\left[ \mathcal{L} - N^{-1} \sqrt{\hat{d}} \sqrt{d}^T \right] \hat{\theta} = \tilde{\lambda} \hat{\theta},
\]

(3.4)

where \( \mathcal{L} = D^{-1/2} A D^{-1/2} \) is the graph Laplacian matrix.

Significance 1. Theorem 5 allows us to interpret the graph Laplacian as the empirical \( \tilde{\mathcal{M}}(\eta,\mathcal{G}_n) \) under degree-adaptive indicator basis choice for the \( \eta \) shape function. Our technique provides a completely nonparametric statistical derivation of an algorithmic spectral graph analysis tool. The plot of \( \tilde{\lambda}_k \) versus \( k \) can be considered as a “raw periodogram” analogue for graph data analysis.

3.2 Diffusion Map

We provide a statistical derivation of Coifman’s diffusion map [Coifman and Lafon 2006] algorithm, which hinges upon the following key result.

**Theorem 6.** The empirical GraField admits the following vertex-domain spectral diffusion decomposition at any finite time \( t \)

\[
\frac{\tilde{p}(t,y|x;\mathcal{G}_n)}{\tilde{p}(y;\mathcal{G}_n)} = 1 + \sum_k \tilde{\lambda}_k \tilde{\phi}_k(x;F) \tilde{\phi}_k(y;F),
\]

(3.5)

where \( \tilde{\phi}_k = D_p^{-1/2} u_k \), \( u_k \) is the \( k \)th eigenvector of the Laplacian matrix \( \mathcal{L} \), \( (\phi_k \circ F)(\cdot) \) is abbreviated as \( \phi_k(\cdot;F) \), \( \tilde{p}(y|x;\mathcal{G}) = \mathcal{T}(x,y) \), and \( \mathcal{T} = D^{-1} A \) is the transition matrix of a random walk on \( \mathcal{G} \) with stationary distribution \( \tilde{p}(y;\mathcal{G}_n) = \frac{d(y;\mathcal{G}_n)}{N} \).

Replacing the estimated coefficients from Theorem 5 into (2.4) yields \( \tilde{\phi}_k = D_p^{-1/2} u_k \), where \( u_k \) is the \( k \)th eigenvector of the Laplacian matrix \( \mathcal{L} \), immediately leads to the following vertex-domain spectral decomposition result of the empirical GraField:

\[
\frac{\tilde{p}(y|x;\mathcal{G})}{\tilde{p}(y;\mathcal{G})} = 1 + \sum_k \tilde{\lambda}_k \tilde{\phi}_k(x) \tilde{\phi}_k(y),
\]

(3.6)

For an alternative proof of the expansion (3.6) see Appendix section of Coifman and Lafon (2006) by noting \( \tilde{\phi}_k \) are the right eigenvectors of random walk Laplacian \( \mathcal{T} \).

Significance 2. In light of Theorem 6, define diffusion map coordinates at time \( t \) as the mapping from \( x \) to the vector

\[
x \mapsto \left( \lambda_1^t \phi_1(x;F), \ldots, \lambda_k^t \phi_k(x;F) \right), \quad x \in \{1,2,\ldots,n\},
\]
which can be viewed as an approximate ‘optimal’ Karhunen-Loève representation basis and thus can be used for non-linear embedding of graphs. Define diffusion distance, a measure of similarity between two nodes of a graph, as the Euclidean distance in the diffusion map space

\[ D^2_t(x, x') = \sum_{j \geq 1} \lambda_j t \{ \phi_j(x; F) - \phi_j(x'; F) \}^2. \]  

(3.7)

This procedure is known as diffusion map, which has been extremely successful tool for manifold learning\textsuperscript{2}. Our approach provides an additional insight and justification for the diffusion coordinates by interpreting it as the strength of connectivity profile for each vertex, thus establishing a close connection with empirical GraField.

### 3.3 Modularity Spectral Analysis

**Theorem 7.** To approximate the KL graph basis \( \phi_k = \sum_j \theta_{jk} \eta_j \), choose \( \eta_j(u) = \mathbf{1}(u_{j-1} < u \leq u_j) \) to be the characteristic function satisfying

\[ \int_0^1 \eta_j(u) \, du = \int_0^1 \eta_j^2(u) \, du = p(j; G). \]

Then the corresponding empirically estimated spectral graph equation (2.9) can equivalently be reduced to the following generalized eigenvalue equation in terms of the matrix \( \mathcal{B} = A - N^{-1}dd^T \)

\[ \mathcal{B} \alpha = \lambda D \alpha. \]  

(3.8)

**Significance 3.** The matrix \( \mathcal{B} \), known as modularity matrix, was introduced by Newman (2006) from an entirely different motivation. Our analysis reveals that the Laplacian and Modularity based spectral graph analyses are equivalent in the sense that they inherently use the same underlying basis expansion (one is a rescaled version of the other) to approximate the optimal graph bases.

**Remark 2.** Solutions (eigenfunctions) of the GraField estimating equation based on the G-matrix under the proposed specialized nonparametric approximation scheme provides a systematic and unified framework for spectral graph analysis. As an application of this general formulation, we have shown how one can synthesize the well-known Laplacian, diffusion map, and modularity spectral algorithms and view them as “empirical” spectral graph analysis methods. It is one of those rare occasions where one can witness the convergence of statistical, algorithmic and geometry-motivated computational models.

\textsuperscript{2}Manifold learning: Data-driven learning of the “appropriate” coordinates to identify the intrinsic non-linear structure of high-dimensional data. We claim the concept of GraField allows decoupling of the geometrical aspect from the probability distribution on the manifold.
4 Smoothed Spectral Graph Analysis

Smoothness is a universal requirement for constructing credible nonparametric estimators. Spectral graph analysis is also no exception. An improved smooth version of raw-empirical spectral graph techniques will be discussed, revealing a simple and straightforward statistical explanation of the origin of regularized Laplacian techniques.

4.1 High-dimensional Undersampled Regime

Recall from Theorem 4 that the generalized matrix eigenvalue equation (2.6) depends on the unknown network and vertex probability mass functions. This leads us to the question of estimating the unknown distribution \( P = (p_1, p_2, \ldots, p_n) \) (support size = size of the graph = \( n \)) based on \( N \) sample, where \( N = \sum_{i=1}^{n} d_i = 2|E| \). Previously (Theorems 5-7) we have used the unsmoothed maximum likelihood estimate (MLE) \( \tilde{p}(x; G) \) to construct our empirical spectral approximation algorithms, which is the unique minimum variance unbiased estimator. Under standard asymptotic setup, where the dimension of the parameter space \( n \) is fixed and the sample size \( N \) tends to infinity, the law of large numbers ensures optimality of \( \tilde{p} \). As a consequence, empirical spectral analysis techniques are expected to work quite well for dense graphs.

Estimation of probabilities from sparse data. However, the raw \( \tilde{p} \) is known to be strictly sub-optimal (Witten and Bell, 1991) and unreliable in the high-dimensional sparse-regime where \( N/n = O(1) \) (i.e., when parameter dimension and the sample size are comparably large). This situation can easily arise for modern day large sparse graphs where the ratio \( N/n \) is small and there are many nodes with low degree, as is the case of degree sparsity. The naive MLE estimator can become unacceptably noisy (high variability) due to the huge size and sparse nature of the distribution. In order to reduce the fluctuations of “spiky” empirical estimates, some form of “smoothing” is necessary. The question remains: How to tackle this high-dimensional discrete probability estimation problem, as this directly impacts the quality of our nonparametric spectral approximation.

My main purpose in the next section is to describe one such promising technique for smoothing raw-empirical probability estimates, which is flexible and in principle can be applied to any sparse data.

4.2 Spectral Smoothing

We seek a practical solution for circumventing this problem that lends itself to fast computation. The solution, that is both the simplest and remarkably serviceable, is the Laplace/Additive smoothing (Laplace, 1951) and its variants, which excel in sparse regimes (Fienberg and Holland, 1973, Witten and Bell, 1991). The MLE and Laplace estimates of the discrete distribution \( p(j; G_n) \) are respectively given by

Raw-empirical MLE estimates:

\[
\tilde{p}(j; G_n) = \frac{d_j}{N};
\]
Smooth Laplace estimates: 
\[ \hat{p}_\tau(j; G_n) = \frac{d_j + \tau}{N + n\tau} \quad (j = 1, \ldots, n). \]

Note that the smoothed distribution \( \hat{p}_\tau \) can be expressed as a convex combination of the empirical distribution \( \tilde{p} \) and the discrete uniform distribution \( 1/n \)
\[ \hat{p}_\tau(j; G_n) = \frac{N}{N + n\tau} \tilde{p}(j; G_n) + \frac{n\tau}{N + n\tau} \left( \frac{1}{n} \right), \quad (4.1) \]
which provides a Stein-type shrinkage estimator of the unknown probability mass function \( p \). The shrinkage significantly reduces the variance, at the expense of slightly increasing the bias.

**Choice of \( \tau \).** The next issue is how to select the “flattening constant” \( \tau \). The following choices of \( \tau \) are most popular in the literature:
\[
\tau = \begin{cases} 
1 & \text{Laplace estimator;} \\
1/2 & \text{Krichevsky–Trofimov estimator;} \\
1/n & \text{Perks estimator;} \\
\sqrt{N/n} & \text{Minimax estimator (under \( L^2 \) loss).}
\end{cases}
\]

**Note 5.** Under increasing-dimension asymptotics, this class of estimator is often difficult to improve without imposing additional smoothness constraints on the vertex probabilities; see Bishop et al. (2007, Chapter 12). The latter may not be a valid assumption as nodes of a graph offer no natural order in general.

With this understanding, smooth generalizations of empirical spectral graph techniques will be discussed, which have a close connection with recently proposed spectral regularized techniques.

### 4.3 Type-I Regularized Graph Laplacian

Construct \( \tau \)-regularized smoothed empirical \( \eta_{j; \tau} \) basis function by replacing the amplitude \( p^{-1/2}(j) \) by \( \hat{p}_\tau^{-1/2}(j) \) following (4.1). Incorporating this regularized trial basis, we have the following modified \( G \)-matrix based linear algebraic estimating equation (2.6):
\[
\sum_j \theta_{jk} \left[ \frac{\tilde{p}(j, k)}{\sqrt{\hat{p}_\tau(j)}} \sqrt{\hat{p}_\tau(k)} - \sqrt{\hat{p}_\tau(j)} \sqrt{\hat{p}_\tau(k)} - \lambda_k \delta_{jk} \right] = 0. \quad (4.2)
\]

**Theorem 8.** The \( \tau \)-regularized block-pulse series based spectral approximation scheme is equivalent to representing or embedding discrete graphs in the continuous eigenspace of
\[
\text{Type-I Regularized Laplacian} \quad = \quad D_\tau^{-1/2} A D_\tau^{-1/2}, \quad (4.3)
\]
where \( D_\tau \) is a diagonal matrix with \( i \)-th entry \( d_i + \tau \).

**Note 6.** It is interesting to note that this exact regularized Laplacian formula was proposed by Chaudhuri et al. (2012) and Qin and Rohe (2013), albeit from a very different motivation.

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\(^3\)For more details on selection of \( \tau \) see Fienberg and Holland (1973) and references therein.
4.4 Type-II Regularized Graph Laplacian

Theorem 9. Estimate the joint probability \( p(j, k; \mathcal{G}) \) by extending the formula given in (4.1) for the two-dimensional case as follows:

\[
\hat{p}_\tau(j, k; \mathcal{G}) = \frac{N}{N + n\tau} \tilde{p}(j, k; \mathcal{G}) + \frac{n\tau}{N + n\tau} \left( \frac{1}{n^2} \right),
\]

which is equivalent to replacing the original adjacency matrix by \( A_\tau = A + (\tau/n)11^T \). This modification via smoothing in the estimating equation (4.2) leads to the following spectral graph matrix

\[
\text{Type-II Regularized Laplacian} = D_\tau^{-1/2} A_\tau D_\tau^{-1/2}.
\]

Note 7. Exactly the same form of regularization of Laplacian graph matrix (4.5) was proposed by Amini et al. (2013) as a fine-tuned empirical solution.

Significance 4. Recently there has been a lot of discussion on how to choose the spectral regularization parameter \( \tau \). Using Davis–Kahan’s theorem, Joseph and Yu (2016) have proposed a data-driven technique called \( \text{DKest} \). Their method involves repeated eigendecomposition of regularized Laplacian matrix (which is a dense matrix) over a grid of values of \( \tau \). There are two major concerns for \( \text{DKest} \): heavy computational burden and theoretical validity (which only holds for stochastic block models and its extensions). In contrast, our analysis provides a strikingly simple recommendation without any additional computational burden (by connecting it to large sparse distribution smoothing), and thus is much easier to construct, implement, and use in practice. Similar to Joseph and Yu (2016), the critical parameter of our theory is the ratio \( N/n \)–the average degree of the nodes, contrary to the previous results (Chaudhuri et al., 2012; Qin and Rohe, 2013) that relied on the minimum degree.

4.5 Google’s PageRank Method

Smoothing of network and vertex probability distributions appearing in generalized matrix equation (2.6) resulted in Type-I and Type-II regularized Laplacian methods. The third possibility is to directly smooth the conditional or transitional probability matrix to develop a regularized version of random walk Laplacian (which we call Type-III regularized Laplacian) method for large sparse graphs.

Smoothing conditional probability function. Consider a random walk on \( \mathcal{G} \) with transition probability \( T(i, j; \mathcal{G}) = \Pr(X_{t+1} = j | X_t = i) \geq 0 \). Note that the smoothing (4.4) can equivalently be represented as

\[
T_\tau(i, j; \mathcal{G}) = \frac{A(i, j; \mathcal{G}) + \tau/n}{d_i + \tau} = (1 - \alpha_\tau)T(i, j; \mathcal{G}) + \alpha_\tau \left( \frac{1}{n} \right),
\]

(4.6)
where the degree-adaptive regularization parameter \( \alpha = \tau (d_i + \tau)^{-1} \). One can construct an equivalent and more simplified (non-adaptive) estimator by directly smoothing each row of \( T \) (as it is a row-stochastic or row-Markov matrix) via Stein-like shrinkage

\[
\mathcal{T}_\alpha = (1 - \alpha)T + \alpha \begin{bmatrix}
1/n & 1/n & \ldots & 1/n \\
\vdots & \vdots & \ddots & \vdots \\
1/n & 1/n & \ldots & 1/n
\end{bmatrix}, \quad 0 < \alpha < 1. \tag{4.7}
\]

Spectral analysis can now proceed on this regularized transition probability matrix (either (4.6) or (4.7)) by substituting empirical transition matrix \( \tilde{T} = D^{-1}A \).

**Significance 5.** The non-adaptive regularized random-walk Laplacian (transition matrix) \( \mathcal{T}_\alpha \) was introduced by Larry Page and Sergey Brin in 1996 (Brin and Page, 1999) and is called the Google’s PageRank matrix. What seems natural enough from our nonparametric smoothing perspective, is in fact known to be highly surprising adjustment—the “Teleportation trick”.

‘Teleporting is the essential distinguishing feature of the PageRank random walk that had not appeared in the literature before’—Vigna (2005).

**Note 8.** The Google’s PageRank matrix (which is different from the empirical random walk Laplacian in an important way) is probably the most famous, earliest, and spectacular example of spectral regularization that was originally introduced to counter the problem of dangling nodes (nodes with no outgoing edges) by “connecting” the graph.

Web is a huge heterogeneous sparse graph where dangling nodes (dead-ends) and disconnected components are quite common. As a result random walk can get stuck, and may cycle around an isolated set of pages. Smoothing allows the random walk to teleport to a web page uniformly at random (or adaptively based on degree-weights) whenever it hits a dead end. The steady state vector describes the long term visit rate—the PageRank score, computed via eigen-decomposition of \( \mathcal{T}_\alpha \).

### 4.6 Other Generalizations

The beauty of our statistical argument is that it immediately opens up several possibilities to construct new types of spectral regularization schemes, which are otherwise hard to guess using previous understanding. Two such promising techniques are discussed here. The first one deals with Stein smoothing with data-driven shrinkage parameter.

**Theorem 10.** Under the sparse asymptotic setup where the domain size \( n \to \infty \) at the same rate as the sample size \( N \), the risk (expected squared-error loss) of smooth add-\( \hat{\tau} \) probability estimate \( \hat{p}_{\hat{\tau}} \) (4.1) with the following data-driven choice

\[
\hat{\tau} = \frac{N^2 - \sum_{i=1}^{n} d_i^2}{n \sum_{i=1}^{n} d_i^2 - N^2} \tag{4.8}
\]

\(^4\)From a statistical estimation viewpoint, this can be thought of as a way to escape from the “zero-frequency problem” for discrete probability estimation.
is uniformly smaller than the risk of the unsmoothed MLE estimator \( \tilde{p} = N^{-1}(d_1, \ldots, d_n) \). In addition, the risk of \( \hat{p}_\tau \) is uniformly smaller than the risk of the estimator formed by choosing \( \tau = 1/2 \).

For proof one can use the technique described in [Fienberg and Holland (1973)]. As a consequence of this result, we can further improve the spectral regularization algorithm by selecting \( \tau \) in a data-driven way, with no extra computation.

While the Laplace or additive smoothing performs well in general, there are situations where they perform poorly ([Gale and Church (1994)]). The Good-Turing estimator ([Good (1953)]) is often the next best choice which is given by

\[
\hat{p}_{GT}(i; G) = \frac{\varpi_{d_i+1}}{\varpi_{d_i}} \cdot \frac{d_i}{N},
\]

where \( \varpi_k \) denotes the number of nodes with degree \( k \). An excellent discussion on this topic can be found in [Orlitsky et al. (2003)]. One can plug in the estimate (4.9) into the equation (4.2) to generate new spectral graph regularization technique.

**Significance 6.** We wish to emphasize that our novelty lies in addressing the open problem of obtaining a rigorous interpretation and extension of spectral regularization. To the best of our knowledge this is the first work that provides a more formal and intuitive understanding of the origin of spectral regularization. We have shown how the regularization naturally arises as a consequence of high-dimensional discrete data smoothing. In addition, this point of view allows us to select appropriate regularization parameter \( \tau \) with no additional computation.

## 5 Application to Graph Regression

We study the problem of graph regression as an interesting application of the proposed nonparametric spectral analysis algorithm. Unlike traditional regression settings, here, one is given \( n \) observations of the response and predictor variables over the graph. The goal is to estimate the regression function by properly taking into account the underlying graph-structured information along with the set of covariates.

**Meuse Data Modeling.** We apply our frequency domain graph analysis to address the spatial prediction problem. Fig 2 describes the Meuse data set, a well known geostatistical dataset. There is a considerable spatial pattern one can see from Fig 2. We seek to estimate a smooth regression function of the dependent variable \( Y \) (zinc concentration in the soil) via generalized spectral regression that can exploit this spatial dependency. The graph was formed according to the geographic distance between points based on the spatial locations of the observations. We convert spatial data into signal supported on the graph by connecting two vertices if the distance between two stations is smaller than a given coverage radius. The maximum of the first nearest neighbor distances is used as a coverage radius to ensure at least
Figure 2: The Meuse dataset consists of \( n = 155 \) observations taken on a support of \( 15 \times 15 \) m from the top \( 0-20 \) cm of alluvial soils in a \( 5 \times 2 \) km part of the right bank of the floodplain of the the river Meuse, near Stein in Limburg Province (NL). The dependent variable \( Y \) is the zinc concentration in the soil (in mg kg\(^{-1}\)), shown in the leftmost figure. The other three variables, flooding frequency class (\( 1 = \) once in two years; \( 2 = \) once in ten years; \( 3 = \) one in 50 years), distance to river Meuse (in metres), and soil type (\( 1 = \) light sandy clay; \( 2 = \) heavy sandy clay; \( 3 = \) silty light clay), are explanatory variables.

one neighbor for each node. Fig 3(C) shows the sizes of neighbours for each node ranging from 1 to 22. Three nodes (\# 82, 148, and 155) have only 1 neighbour; additionally one can see a very weakly connected small cluster of three nodes, which is completely detached from the bulk of the other nodes. The reason behind this heterogeneous degree distribution (as shown in Fig 3) is the irregular spatial pattern of the Meuse data.

We model the relationship between \( Y \) and spatial graph topology by incorporating nonparametrically learned spectral representation basis. Thus, we expand \( Y \) in the eigenbasis of \( \mathcal{C} \) and the covariates for the purpose of smoothing, which effortlessly integrates the tools from harmonic analysis on graphs and conventional regression analysis. The model (5.1) described in the following algorithm simultaneously promotes spatial smoothness and sparsity.

Algorithm 2. *Nonparametric Spectral Graph Regression*

**Step 1.** Input: We observe \( \{y_i; x_{i1}, \ldots, x_{in}\} \) at vertex \( i \) of the graph \( \mathcal{G} = (V, A) \) with size \( |V| = n \). The regularization parameters \( \tau \).

**Step 2.** Construct \( \tau \)-regularized block-pulse shape functions \( \eta_{j,\tau} = \hat{p}_{j,\tau}^{-1/2} \mathbb{I}(u_{j-1} < u \leq u_j) \) for \( j = 1, \ldots, n \).

**Step 3.** Compute the smoothed \( \textit{G-Matrix} \) with respect to trial bases \( \{\eta_{k,\tau}\}_{1 \leq k \leq n} \)

\[
\mathcal{M}_\tau[j, k; \eta, \mathcal{G}] = \left< \eta_{j,\tau}, \int_0^1 (\mathcal{C}_n - 1) \eta_{k,\tau} \right>_{L^2[0, 1]} \quad \text{for } j, k = 1, \ldots, n.
\]
Step 4. Construct smooth graph Fourier basis

\[ \tilde{\phi}_{k,\tau}(u) = \sum_{j=1}^{n} u_{jk} \eta_j, \text{ for } k = 1, \ldots, n - 1, \]

where \( M = U \Lambda U^T = \sum_k u_k \mu_k u_k^T \), and \( u_{ij} \) are the elements of the singular vector \( U = (u_1, \ldots, u_n) \). Construct spectral basis matrix \( \Phi = [\tilde{\phi}_{1,\tau}, \ldots, \tilde{\phi}_{k,\tau}] \in \mathbb{R}^{n \times k} \) for the graph \( G \).

Step 5. Construct combined graph regressor matrix \( X_G = [\Phi; X] \), where \( X = [X_1, \ldots, X_p] \in \mathbb{R}^{n \times p} \) is the matrix of predictor variables.

Step 6. Solve for \( \beta_G = (\beta_\Phi, \beta_X)^T \)

\[ \hat{\beta}_G = \underset{\beta_G \in \mathbb{R}^{k+p}}{\text{argmin}} \| y - X_G \beta_G \|^2_2 + \lambda \| \beta_G \|_1. \] (5.1)

Algorithm 2 extends traditional regression to data sets represented over a graph. The proposed frequency domain smoothing algorithm efficiently captures the spatial graph topology via the spectral coefficients \( \hat{\beta}_\Phi \in \mathbb{R}^k \) and can be interpreted as covariate-adjusted discrete graph Fourier transform of the response variable \( Y \). The \( \ell_1 \) sparsity penalty automatically selects the coefficients with largest magnitudes thus provides compression.

The following table shows that incorporating the spatial correlation in the baseline unstructured regression model using spectral orthogonal basis functions (which are estimated from the spatial graph with \( k = 25 \)) boosts the model fitting from 62.78% to 80.47%, which is an improvement of approximately 18%.
Here $\tilde{\Phi}_0$, $\tilde{\Phi}_I$ and $\tilde{\Phi}_{II}$ are the graph-adaptive piecewise constant orthogonal basis functions derived respectively from the ordinary, Type-I regularized, and Type-II regularized Laplacian matrix. Using other forms of regularization the performance does not change much, and thus we do not show it here. Our spectral method can also be interpreted as a kernel smoother, where the spatial dependency is captured by the discrete GraField. We finally conclude that extension from traditional regression to graph-structured spectral regression significantly improves the model accuracy.

### 6 Concluding Remarks

What is the “common core” behind all existing spectral graph techniques? Despite half a century of research, it remains one of the most formidable open issues, if not the core problem in modern spectral graph theory. The need for a unified theory become particularly urgent and pressing in the era of “algorithm deluge” in order to systematize the practice of graph data analysis.

As an attempt to shed some light on this previously unasked question, I have introduced a framework for statistical reasoning that appears to offer a complete and autonomous description (totally free from the classical combinatorial or algorithmic linear algebra-based languages) with the intention of leading the reader to a broad understanding of how different techniques interrelate. The prescribed approach brings a fresh perspective by appropriately transforming the spectral problem into a nonparametric approximation and smoothing problem to arrive at new algorithms, as well as both practical and theoretical results. It was a great surprise for me to be able to deduce existing techniques from some underlying basic principles in a self-consistent way. At the end, there is always the hope that a comprehensive understanding gained through unification will inspire new tools, to attack some of the important open problems in this area.

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To further demonstrate the potential application of smooth spectral graph algorithms, in this supplementary section we discuss the community detection problem that seeks to divides nodes into into $k$ groups (clusters), with larger proportion of edges inside the group (homogeneous) and comparatively sparser connections between groups to understand the large-scale structure of network. Discovering community structure is of great importance in many fields such as LSI design, parallel computing, computer vision, social networks, and image segmentation.

**Graph Clustering**

In mathematical terms, the goal is to recover the graph signals (class labels) $y : V \mapsto \{1, 2, \ldots, k\}$ based on the connectivity pattern or the relationship between the nodes. Representation of graph in the spectral or frequency domain via the nonlinear mapping $\Phi : G(V, E) \mapsto \mathbb{R}^m$ using discrete KL basis of density matrix $\mathcal{C}$ as the co-ordinate is the most important learning step in the community detection. This automatically generates spectral features $\{\phi_{1i}, \ldots, \phi_{mi}\}_{1 \leq i \leq n}$ for each vertex that can be used for building the distance or similarity matrix to apply k-means or hierarchical clustering methods. In our examples, we will apply k-means algorithm in the spectral domain, which seeks to minimizing the within-cluster sum of squares. In practice, often the most stable spectral clustering algorithms determine $k$ by spectral gap: $k = \text{argmax}_j |\lambda_j - \lambda_{j+1}| + 1$.

**Algorithm 3. Nonparametric Spectral Graph Partitioning**

1. Input: The adjacency matrix $A \in \mathbb{R}^{n \times n}$. Number of clusters $k$. The regularization parameter $\tau$.

2. Estimate the top $k - 1$ spectral connectivity profile for each node $\{\tilde{\phi}_{1i;\tau}, \ldots, \tilde{\phi}_{(k-1)i;\tau}\}$ using Algorithm 2. Store it in $\Phi \in \mathbb{R}^{n \times k-1}$.

3. Apply k-means clustering by treating each row of $\Phi$ as a point in $\mathbb{R}^{k-1}$.

4. Output: The cluster assignments of $n$ vertices of the graph $C_1, \ldots, C_k$. 

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S–1
In addition to graph partitioning, the spectral ensemble \( \{\lambda_k, \phi_k\}_{1 \leq k \leq m} \) of \( G \) contain a wealth of information on the graph structure. For example, the quantity \( 1 - \tilde{\lambda}_1(G; \eta) \) for the choice of \( \{\eta_k\} \) to be normalized top hat basis (3.1), is referred to as the algebraic connectivity, whose magnitude reflects how well connected the overall graph is. The kmeans clustering after spectral embedding \( \{\tilde{\phi}_j(G; \eta)\}_{1 \leq j \leq k-1} \) finds approximate solution to the NP-hard combinatorial optimization problem based on the normalized cut (Shi and Malik, 2000) by relaxing the discreteness constraints into one that is continuous (sometimes known as spectral relaxation).

**Data and Results.** We investigate four well-studied real-world networks for community structure detection based on 7 variants of spectral clustering methods.

**Example A** [Political Blog data, Adamic and Glance (2005)] The data, which contains 1222 nodes and 16,714 edges, were collected over a period of two months preceding the U.S. Presidential Election of 2004 to study how often the political blogs refer to one another. The linking structure of the political blogosphere was constructed by identifying whether a URL present on the page of one blog references another political blog (extracted from blogrolls). Each blog was manually labeled as liberal or conservative by Adamic and Glance (2005), which we take as ground truth. The goal is to discover the community structure based on these blog citations, which will shed light on the polarization in political blogs.

Table 1 shows the result of applying the spectral graph clustering algorithm on this political web-blog data. The un-regularized Laplacian performs very poorly, whereas as both type-I/II regularized versions give significantly better results. The misclassification error drops from 47.95% to 4.7% because of regularization. To better understand why regularization plays a vital role, consider the degree distribution of the web-blog network as shown in the bottom panel of Figure 2. It clearly shows the presence of a large number of low-degree nodes, which necessitates the smoothing of high-dimensional discrete probability \( p_1, \ldots, p_{1222} \). Thus, we perform the kmeans clustering after projecting the graph in the Euclidean space spanned by Laplace smooth KL spectral basis \( \{\tilde{\phi}_{k;\tau}\} \). Regularized spectral methods correctly identify two dense clusters: liberal and conservative blogs, which rarely links to a blog of a different political leaning, as shown in the middle panel of Fig 5.

**Example B** [US College Football, Grivan and Newman (2002)] The American football network (with 115 vertices, 615 edges) depicts the schedule of football games between NCAA Division IA colleges during the regular season of Fall 2000. Each node represents a college team (identified by their college names) in the division, and two teams are linked if they have played each other that season. The teams were divided into 11 “conferences” containing around 8 to 12 teams each, which formed actual communities. The teams in the same conference played more often compared to the other conferences, as shown in the middle panel of Fig 5. A team played on average 7 intra- and 4 inter-conference games in the season. Inter-conference play is not uniformly distributed; teams that are geographically close to one another but belong to different conferences are more likely to play one another than teams.
Table 1: We report % of misclassification error. We compare following seven different Laplacian variants. $K$ denotes the number of communities.

| Data       | K | Laplacian | Type-I Reg. Laplacian | Type-II Reg. Laplacian |
|------------|---|-----------|-----------------------|------------------------|
|            |   |           | $\tau = 1$ | $\tau = 1/2$ | $\tau = \sqrt{N}/n$ | $\tau = 1$ | $\tau = 1/2$ | $\tau = \sqrt{N}/n$ |
| PolBlogs   | 2 |           | 47.95%   | 4.9%   | 4.8%   | 5.4%   | 4.8%   | 4.7%   | 5.4%   |
| Football   | 11 |          | 11.3%   | 7.83% | 6.96% | 6.96% | 6.96% | 7.83% | 7.83% |
| MexicoPol | 2 |           | 17.14%   | 14.2% | 14.2% | 14.2% | 14.2% | 14.2% | 14.2% |
| Adjnoun   | 2 |           | 13.4%   | 12.5% | 12.5% | 12.5% | 12.5% | 12.5% | 12.5% |

separated by large geographic distances. As the communities are well defined, the American football network provides an excellent real-world benchmark for testing community detection algorithms.

Table 1 shows the performance of spectral community detection algorithms to identify the 11 clusters in the American football network data. The regularization boosts the performance by 3-4%. In particular, $\tau = 1/2$ and $\sqrt{N}/n$ produces the best result for Type-I regularized Laplacian, while $\tau = 1$ exhibits the best performance for Type-II regularized Laplacian.

**Example C** [The Political Network in Mexico, Gil-Mendieta and Schmidt (1996)] The data (with 35 vertices and 117 edges) represents the complex relationship between politicians in Mexico (including presidents and their close associates). The edge between two politicians indicates a significant tie, which can either be political, business, or friendship. A classification of the politicians according to their professional background (1 - military force, 2 - civilians: they fought each other for power) is given. We use this information to compare our 7 spectral community detection algorithms.

Although this is a “small” network, challenges arise from the fact that the two communities cannot be separated easily due to the presence of a substantial number of between-community edges, as depicted in Figs 4 and 5. The degree-sparsity is also evident from Fig 5 (bottom-panel). Table 1 compares seven spectral graph clustering methods. Regularization yields 3% fewer misclassified nodes. Both the type-I and II regularized Laplacian methods for all the choices of $\tau$ produce the same result.

**Example D** [Word Adjacencies, Newman (2006)] This is a adjacency network (with 112 vertices and 425 edges) of common adjectives and nouns in the novel *David Copperfield* by English 19th century writer Charles Dickens. The graph was constructed by Newman.
Figure 4: Mexican political network. Two different colors (golden and blue) denotes the two communities (military and civilians).

(2006). Nodes represent the 60 most commonly occurring adjectives and nouns, and an edge connects any two words that appear adjacent to one another at any point in the book. Eight of the words never appear adjacent to any of the others and are excluded from the network, leaving a total of 112 vertices. The goal is to identify which words are adjectives and nouns from the given adjacency network.

Note that typically adjectives occur next to nouns in English. Although it is possible for adjectives to occur next to other adjectives (e.g., “united nonparametric statistics”) or for nouns to occur next to other nouns (e.g., “machine learning”), these juxtapositions are less common. As expected, Fig 5 (middle panel) shows an approximately bipartite connection pattern among the nouns and adjectives.

A degree-sparse (skewed) distribution is evident from the bottom right of Fig 5. We apply the seven spectral methods and the result is shown in Table 1. The traditional Laplacian yields a 13.4% misclassification error for this dataset. We get better performance (although the margin is not that significant) after spectral regularization via Laplace smoothing.

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Figure 5: The columns denote the 4 datasets corresponding to the political blog, US college football, politicians in Mexico, and word adjacencies networks. The first two rows display the un-ordered and ordered adjacency matrix, and the final row depicts the degree distributions.

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