

# Computational Graph Theory in the Twenty-First Century

Sawyer Jack Robertson

[sawyerrobertson.xyz](http://sawyerrobertson.xyz)

In the 1980s and 1990s, *computational graph theory* was a fashionable umbrella term for topics such as the analysis of algorithms involving graphs and computer-assisted proofs in combinatorial graph theory (see, for example, the book collection [24]), yet the term itself has since waned in popularity. Over the past few years, my body of work has aimed to deliver a principled, fresh perspective on this topic by combining methods and problems from areas such as random graph theory (see [Section 1](#)), graph-based algorithms in data science (see [Section 2](#)), and geometric graph theory (see [Section 3](#)). This research program is driven by my fascination with graphs as mathematical objects that are simultaneously very simple (a graph is a collection of abstract points and some distinguished pairwise relationships between them) and deeply expressive in their ability to capture the structure of complex systems.

During my Ph.D., I have been grateful to be supported and mentored by my advisors Fan Chung and Alex Cloninger. These two professors have provided complementary perspectives ranging from combinatorics and spectral graph theory in the former case to signal processing and machine learning in the latter. As I look to the next phase of my career, I envision this program continuing to evolve and expand in exciting new directions.

## 1 Statistical and Markovian random graph theory

I am interested in random graphs primarily for two reasons: first, for their role in analyzing and benchmarking the performance of graph-based algorithms emerging from data science applications; and second, out of my interest in *Markovian* random graph models and the analysis of such models using techniques from other areas of mathematics. My work in this area primarily focuses on concentration inequalities for matrix-valued statistics of random graphs (see [Section 1.1](#)) and mixing time analyses for stochastically evolving graphs (see [Section 1.2](#)).

### 1.1 Concentration inequalities for matrix-valued statistics of random graphs

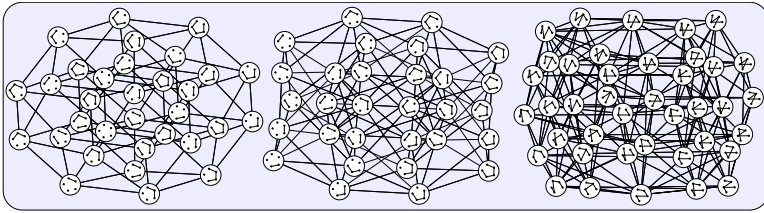
*Spectral clustering* is a widely used method for identifying clusters in graph-structured data, and is loosely described as follows [20]. Given a weighted graph  $G = (V, E, w)$  with  $n$  vertices, one constructs the graph Laplacian matrix  $L = D - W$ , where  $W$  is the weighted adjacency matrix of  $G$  and  $D$  is the diagonal degree matrix with entries  $D_{ii} = \sum_j W_{ij}$ . The leading eigenvectors of  $L$  are then used to embed the vertices of the graph into a lower-dimensional space, where traditional clustering algorithms (e.g.,  $k$ -means) can be applied to identify clusters.

To analyze these methods from a statistical standpoint, various random graph models have been designed to simulate environments conducive to data clustering tasks, and it is of interest to certify that spectral techniques can recover the ground truth information with high probability. These include the well-known *stochastic block models* and so-called *information-plus-noise models*, which consider randomly weighted geometric graphs. There is a rich history on this topic in the statistics literature (see, for starters, [3, 7, 13]).

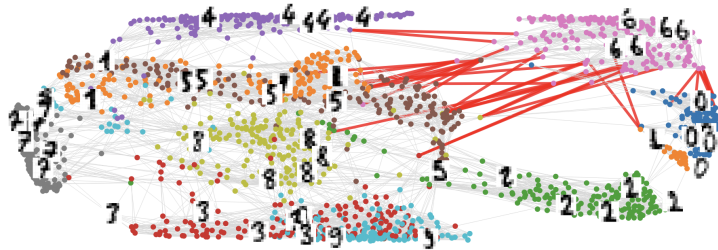
One variant of interest is *inhomogeneous Erdős-Rényi-type signed graphs*, which are random graphs where each pair of vertices is assigned an edge and a positive or negative sign according to some probability distribution. These models are useful for studying networks with both positive and negative relationships, such as social networks with friendships and rivalries. In [14], I established operator norm concentration inequalities for adjacency and Laplacian matrices of inhomogeneous Erdős-Rényi-type signed graphs, providing insights into the consistency of spectral community detection techniques for signed graphs.

In [12] (joint with D. Kohli, G. Mishne, and A. Cloninger), within the context of a manifold learning algorithm detailed at greater length in [Section 2.2](#), I also pursued this theme by analyzing the concentration of graph Laplacians arising from randomized information-plus-noise models and in doing so provided theoretical foundations for robust manifold learning. In particular, I considered a model consisting of a dataset  $\{X_i\}_{i=1}^n$  given by  $X_i = y_i + Z_i$ , where  $\{y_i\}_{i=1}^n$  are “clean” points on a data manifold and  $\{Z_i\}_{i=1}^n$  are independent sub-Gaussian noise vectors. I proved that under certain conditions on the noise distribution and the kernel used to construct the corresponding Laplacian matrix, the noisy graph Laplacian  $L_{\text{noisy}}$  concentrates to the clean graph Laplacian  $L_{\text{clean}}$  with high probability as  $n \rightarrow \infty$ , and hence by Weyl’s inequality and the Davis-Kahan theorem, so do the corresponding eigenvalues and eigenvectors. This result was instrumental in establishing theoretical guarantees for the robustness of our tangent space estimation method.

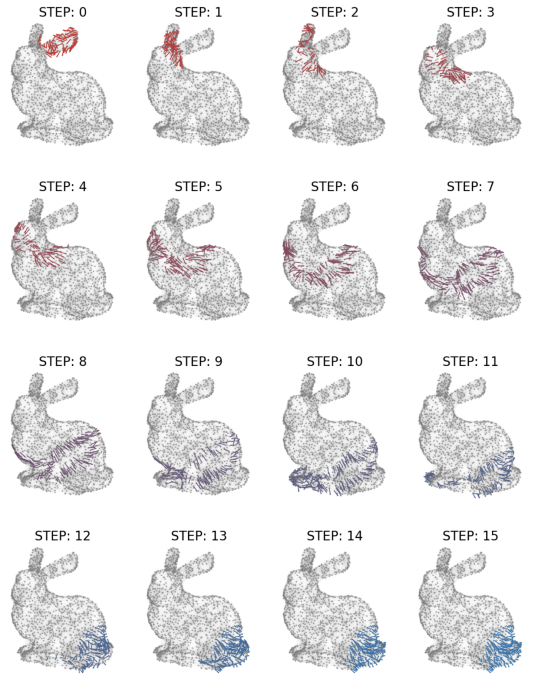
**Theorem 1.1** (Informal statement of eigenvector stability [12]). *Let  $\{y_i\}_{i=1}^n$  be fixed with  $y_i \in \mathbb{R}^d$  and write  $X_i = y_i + Z_i$ , where  $\{Z_i\}_{i=1}^n$  are i.i.d. mean-zero sub-Gaussian noise vectors with variance proxy  $\xi \geq 0$ . Assume that  $\xi = o(1)$  and  $d$  is fixed as  $n \rightarrow \infty$ . Let  $L_{\text{clean}}$  and  $L_{\text{noisy}}$  be the normalized kernel graph Laplacians constructed from  $\{y_i\}_{i=1}^n$  and  $\{X_i\}_{i=1}^n$ , respectively. Then, under certain assumptions on the eigenvalues of  $L_{\text{clean}}$ , the leading  $O(1)$  eigenvectors of  $L_{\text{noisy}}$  converge to those of  $L_{\text{clean}}$  with high probability as  $n \rightarrow \infty$ .*



**Figure 1.** This figure contains three examples of *state graphs*, which are used to model the state spaces of stochastically evolving graph processes. The nodes correspond to labeled subgraphs of a host graph  $\mathcal{H}$ , and the links appear whenever it is possible to transition between the subgraphs according to the process under consideration. From left to right: host graph  $\mathcal{H} = C_5$  according to a simple edit process of adding/deleting edges at random (a hypercube); host graph  $\mathcal{H} = C_5$  corresponding to the Moran forest process of adding/deleting groups of edges in tandem; host graph given by the HouseX graph, with respect to the Glauber dynamics process on its spanning trees.



**Figure 2.** This figure contains a graph with vertices corresponding to the entries of a small digits dataset [1]. Edges are included whenever two images are close in Euclidean distance. We seek to classify images of the digit 6 from images of all other digits. The reference measure  $\mu$  is uniform on the sixes with their images overlaid in the figure, and the reference measure  $\nu$  is uniform on those vertices with images overlaid as well. We highlight in red edges that are cut according to the program  $C_1(\mu, \nu)$ .



**Figure 3.** By defining a notion of *minimum cost parallel transport* between vector fields on a geometric graph [17], we introduced an algorithm for vector field interpolation on graphs. Here, we illustrate such an interpolation between vector fields defined on the Stanford bunny [22].

## 1.2 New directions in stochastically evolving graphs

*Stochastically evolving graphs* appear when the structure of a graph changes over time according to some stochastic, usually Markovian, process. In theoretical computer science, these models appear frequently in the form of sampling algorithms for structures such as matchings, spanning trees, and colorings. In applied settings, these models are useful for studying dynamic networks, such as social networks, communication networks, and biological networks (for the sake of brevity, I omit a literature review here). One way to view an evolving graph model is to think of it as a random walk on a state space consisting of graphs; we model these spaces as so-called *state graphs* (see Fig. 1).

Often a key objective in the analysis of these models is the *mixing time* of the underlying Markov chain, which measures how quickly the distribution converges to its stationary distribution. Understanding mixing times is crucial for designing efficient algorithms and for characterizing the long-term behavior of dynamic networks. Classical estimates relate the mixing time of an ergodic, reversible Markov chain  $P$  to its largest nontrivial eigenvalue, thereby motivating the investigation of the spectral decomposition of Markov kernels as a means to certify their mixing times. In many cases, however, the state space of the Markov chain is combinatorial in nature, making direct spectral analysis very challenging.

In [4] (joint with F. Chung), I introduced a model for dynamically evolving graphs based on random edits. Specifically, I considered a random walk on the subgraphs of a fixed graph  $G$  where at each step a randomly chosen “edit” (e.g., adding/removing one edge, or compound edits affecting many edges) is applied. By showing that the edits form a semigroup known as a *left regular band*, we derived closed-form formulas for the eigenvalues of the associated transition probability matrix and sharp mixing time estimates. This highly general framework extends to models such as the Moran forest model (see [2]) and random intersection graph processes. Below I provide an informal statement of one of our main results.

**Theorem 1.2** (Informal statement, eigenvalues of compound edit processes [4]). *Let  $G = (V, E)$  denote a fixed host graph and let  $\mathbf{A}$  be a given set of edits (defined as idempotent maps on  $2^E$ ). Let  $w \in \mathbb{R}^{\mathbf{A}}$  be a given probability distribution on  $\mathbf{A}$ . Consider the random walk obtained as follows: start with a labeled subgraph  $G_0$  of  $G$ , and at each time  $t \geq 1$ , sample an edit  $x \sim w$  and write  $G_t = xG_{t-1}$ . Denote the transition probability matrix of this process by  $\mathcal{P}$ . Then  $\mathcal{P}$  is diagonalizable and its eigenvalues are related to a certain join semilattice associated to  $G$  and  $\mathbf{A}$ , and can be computed in closed form.*

## Future directions

- The framework I developed in [4] constructs a wide variety of stochastic processes on graphs that are rapidly mixing. Can we use this finding to design new sampling algorithms for combinatorial structures, or diffusion-based generative graph models?
- If  $G$  is a fixed graph and we retain each edge with probability  $p$  (or  $k = o(n)$  neighbors of each vertex), how small can  $p$  (or  $k$ ) be taken while ensuring that the low-frequency eigenvectors still approximate those of  $G$  with high probability as the number of vertices grows? These are related to *randomized near neighbor graphs* (see [11]).

## 2 Graph-based methods in data science

Graphs have been used to develop algorithms and models for a variety of data science tasks, including clustering, classification, and dimensionality reduction. My work in this area primarily focuses on optimal transport and graph-based semi-supervised learning (see [Section 2.1](#)), and geometric data analysis (see [Section 2.2](#)).

### 2.1 Optimal transport and graph-based SSL

*Optimal transport* (OT) is a powerful tool for comparing and analyzing probability distributions, with applications in machine learning, computer vision, and economics. For a weighted graph  $G = (V, E, w)$ , let  $\mathcal{P}(V)$  denote the set of probability density vectors supported on  $V$ . For  $\mu, \nu \in \mathcal{P}(V)$ , the *1-Wasserstein distance*  $W_1(\mu, \nu)$  is given by

$$W_1(\mu, \nu) = \inf_{\pi \in \Pi(\mu, \nu)} \sum_{x, y \in V} d_G(x, y) \pi(x, y), \quad (1)$$

where  $\Pi(\mu, \nu)$  is the set of couplings between  $\mu$  and  $\nu$ , and  $d_G(x, y)$  is the shortest path distance between vertices  $x$  and  $y$  (which by convention is weighted). In the graph setting, the program [Eq. \(1\)](#) is equivalent to the following minimum-cost flow problem known as the *Beckmann problem*:

$$W_1(\mu, \nu) = \min_{\substack{J: E \rightarrow \mathbb{R} \\ \text{div}(J) = \mu - \nu}} \sum_{e \in E} w_e |J(e)|.$$

Here,  $J$  is a flow on the edges of the graph,  $w_e$  denotes the edge weights, and  $\text{div}(J)$  is the divergence of the flow at each vertex defined by the action of the vertex-edge oriented incidence matrix. In [19] (joint with Z. Wan and A. Cloninger), I explored connections between  $W_1(\mu, \nu)$  and extensions of the Beckmann problem to include  $p$ -norm costs on flows, which we termed  $p$ -Beckmann problems. Specifically, if  $p \in [1, \infty]$ , we defined

$$B_p(\mu, \nu) = \min_{\substack{J: E \rightarrow \mathbb{R} \\ \text{div}(J) = \mu - \nu}} \sum_{e \in E} w_e |J(e)|^p, \quad \text{if } p < \infty, \text{ and } \quad B_\infty(\mu, \nu) = \min_{\substack{J: E \rightarrow \mathbb{R} \\ \text{div}(J) = \mu - \nu}} \max_{e \in E} |J(e)|.$$

I developed a duality theory for these problems and demonstrated their utility in various clustering tasks. Moreover, I showed that the 2-Beckmann distance generalizes effective resistance on graphs to the probability simplex and linked it to random walks and homogeneous Sobolev seminorms.

The  $p$ -Beckmann problems also served as the basis for a graph-based *semi-supervised learning* (SSL) method introduced in [16] (joint with C. Holtz, Z. Wan, G. Mishne, and A. Cloninger). SSL, generally speaking, aims to use both labeled and unlabeled data to improve model performance. Our proposed learning method balances edge sparsification with class separation (see [Fig. 2](#)); specifically, we considered the following  $p$ -conductance program between measures  $\mu, \nu \in \mathcal{P}(V)$ :

$$C_p(\mu, \nu) = \min_{\substack{\phi \in \mathbb{R}^V \\ \phi^\top(\mu - \nu) \geq 1}} \sum_{e = \{x, y\} \in E} w_e |\phi(x) - \phi(y)|^p.$$

By using gauge duality (see [10]), we established a relationship between  $C_p(\mu, \nu)$  and  $B_p(\mu, \nu)$ , connecting potentials used in our SSL method to the  $p$ -Beckmann problems (see [Theorem 2.1](#)).

**Theorem 2.1** (Relationships between Beckmann and Conductance programs [16]). *Let  $\mu, \nu \in \mathcal{P}(V)$  be distinct. Then the optimal values of  $C_p$  and  $B_p$  are related as follows:*

$$C_p(\mu, \nu) = \begin{cases} 1/B_{\infty, w^{-1}}(\mu, \nu) & \text{if } p = 1, \\ 1/B_{q, w^{1-q}}(\mu, \nu) & \text{if } p \in (1, \infty) \text{ and } 1/p + 1/q = 1, \\ 1/B_{1, w^{-1}}(\mu, \nu) & \text{if } p = \infty. \end{cases}$$

In particular, if  $G = (V, E)$  has unit weights, then  $C_\infty(\mu, \nu) = 1/W_1(\mu, \nu)$  and

$$C_2(\mu, \nu)^2 = 1/B_2(\mu, \nu)^2 = 1/(\mu - \nu)^\top L^\dagger (\mu - \nu),$$

where  $L^\dagger$  is the Moore-Penrose inverse of  $L$ .

## 2.2 Geometric data analysis

In many data science applications, one encounters data that lies on or near a low-dimensional manifold embedded in a high-dimensional ambient space. Capturing the geometric structure of such data is crucial for effective analysis and learning. One of the specific subtasks in this area is *tangent space estimation*, which involves estimating the tangent spaces of the manifold at various points based on the graph structure. Well known methods such as *local PCA* [21], which estimates tangent spaces by performing PCA on the features in each neighborhood of a vertex in a weighted graph  $G = (V, E, w)$ , can be sensitive to noise and perturbations in the data and in such settings lead to inaccurate tangent space estimates.

Based on empirical observations that low-frequency eigenvectors of graph Laplacians are more robust to noise than the eigenvectors appearing deeper in the spectrum, in [12] (joint with D. Kohli, G. Mishne, and A. Cloninger), we developed a spectral method for robust tangent space estimation on noisy manifolds. Our method, termed **LEGO**, proceeds by orthogonalizing the gradients of the low-frequency eigenvectors of the graph Laplacian to estimate the tangent spaces at each vertex. Specifically, for each vertex  $i \in V$ , we compute the gradients  $\nabla \phi_j(x_i)$  of the first  $m$  eigenvectors  $\{\phi_j\}_{j=1}^m$  of the graph Laplacian and then apply a localized orthogonalization procedure to obtain an estimate of the tangent space  $T_{x_i}\mathcal{M}$ . We provided two theoretical arguments to support our empirical observations: (i) a differential geometric analysis on tubular neighborhoods showing that eigenfunctions with large gradients in noise directions lie deeper in the spectrum; (ii) a random matrix analysis proving the noisy graph Laplacian concentrates to the clean operator w.h.p. in certain noise regimes, so low-frequency eigenvectors (and their gradients) are noise stable (see [Theorem 1.1](#)).

### Future directions

- In ongoing work (with C. Holtz, M. Black, and others), I am investigating the relationship between existing notions of edge centrality metrics such as the *betweenness centrality* and *biharmonic distance*. We aim to establish equivalences such as the ones outlined in [Theorem 2.1](#).
- We are also currently working on formalizing guarantees for the observed robustness of the graph cut-based SSL method proposed in [16].

## 3 Geometric graph theory: connections and curvatures

Graphs can be equipped, both intrinsically and extrinsically, with geometric features that capture various properties of the underlying combinatorial structures or data. My work in this area primarily focuses on connection Laplacians (see [Section 3.1](#)) and discrete curvature notions (see [Section 3.2](#)).

### 3.1 Connection Laplacians

One way to incorporate extrinsic geometric information into graph-based frameworks is through the usage of *connection Laplacians*, which are matrices that encode parallel transport operators between vector spaces at each vertex. Specifically, a *connection graph* is a tuple  $(G, \sigma)$  where  $G = (V, E, w)$  is a weighted graph and  $\sigma : E \rightarrow O(d)$  is a *connection* assigning an orthogonal transformation to each edge. The connection Laplacian  $L_\sigma$  is defined as

$$(L_\sigma f)(i) = \sum_{j: \{i,j\} \in E} w_{ij}(f(i) - \sigma_{ij}f(j)), \quad f : V \rightarrow \mathbb{R}^d.$$

Connection Laplacians have been used in various applications, including computer vision, manifold learning, and shape analysis (for brevity I omit a literature review here).

In [5] (joint with A. Cloninger, G. Mishne, A. Oslandsbotn, Z. Wan, and Y. Wang), we studied matrix-valued Dirichlet problems on connection graphs and used their solutions to define connection voltage functions and conductance matrices that extend these otherwise classical notions to the connection setting. These matrices encode the effective conductance between nodes while also reflecting the connection structure. We also extended the notion of effective resistance to connection graphs based on the solution of a Poisson-type problem in a matrix-valued unknown. We proved that  $R_\sigma$  is, up to a structured congruence, the pseudoinverse of the conductance matrix.

In [17] (joint with D. Kohli, G. Mishne, and A. Cloninger), we generalized discrete optimal transport to vector fields on connection graphs by defining the *connection Beckmann problem* as follows:

$$W_1^{\sigma, \lambda}(\alpha, \beta) = \min_{\substack{J: E \rightarrow \mathbb{R}^d \\ \text{div}_\sigma(J) = \alpha - \beta}} \sum_{e \in E} w_e \|J(e)\| + \lambda \|J\|_2^2$$

where  $\text{div}_\sigma$  is the connection divergence operator that incorporates the connection  $\sigma$ . This problem models the optimal parallel transport cost between vector fields  $\alpha, \beta : V \rightarrow \mathbb{R}^d$  on a data manifold. We established feasibility criteria and duality results for the connection Beckmann problem, as well as a relaxed and regularized variant thereof. We demonstrated that our work can be applied to various data science tasks with a geometric component, such as color image processing and directional data analysis (see [Fig. 3](#)).



## 3.2 Discrete curvatures

Curvature is a fundamental concept in differential geometry that quantifies how much a geometric object deviates from being flat at a point. In recent years, there has been rapidly growing interest in developing discrete notions of curvature for graphs and networks, which can provide insights into their structural properties. Various discrete curvature notions have been proposed and studied (for brevity I omit a literature review here).

In [6] (joint with J. A. De Loera, J. Eddy, and J. A. Samper), we studied discrete curvature notions (specifically, resistance curvature [8] and Forman–Ricci curvature [9]) on convex polytopes, proving finiteness and abundance theorems in various dimensions. This marked the first systematic study of discrete curvature notions on polytopal graphs, revealing new connections between combinatorial geometry and discrete curvature. Separately, in [15], I derived explicit formulas for Wasserstein distances and curvatures on trees, and obtained comparison results between different curvature notions. This marked one of only a few papers which develop quantitative comparisons between multiple notions of discrete curvature in one setting.

Finally, in [18] (joint with F. Southerland and E. Surya), we investigated a special class of graphs arising from a notion of curvature of Steinerberger [23]. Specifically, we studied *distance exceptional graphs*, which are graphs where the equation  $Dx = \mathbf{1}$  does not have a solution. Here,  $D$  is the distance matrix of the graph and  $\mathbf{1}$  is the all-ones vector. These graphs appear naturally within the curvature framework of Steinerberger, but are mysterious in many respects. Prior to our work, constructions of these graphs were extremely constrained and poorly understood. We introduced a graph invariant called the *curvature index*, which measures the extent to which a graph deviates from being distance exceptional (and, in particular, vanishes when  $G$  is distance exceptional). In doing so, we generalized a number of known theorems in this field and proved an embedding theorem, stated below.

**Theorem 3.1** (Informal statement of distance exceptional embeddings [18]). *Let  $G$  be any graph, connected or otherwise. Then there exists a distance exceptional graph  $G'$  such that  $G$  is isomorphic to an induced subgraph of  $G'$ . Moreover, if  $G$  satisfies  $\iota(G) < \infty$ , where  $\iota(G)$  is the curvature index of  $G$  (definition omitted), then the embedding can be chosen to be an isometry.*

## 3.3 Future directions

- State graphs (see Fig. 1) provide a rich class of large graphs related to stochastically evolving graph processes (see Section 1.2). Can we characterize their discrete curvature properties and relate them to mixing times of the underlying processes?
- In the Erdős–Rényi random graph  $G(n, p)$ , can we understand the behavior of the curvature index as  $n \rightarrow \infty$ ? What fraction of graphs are distance exceptional?

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