A Review of Spectral Graph With a Focus On Chemical Reaction Networks

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Abstract

Un-directed graphs can be defined as symmetric positive semi-definite matrices via the discreet graph Laplacian matrix. These properties have been exploited to develop a vast array of results that are used to study complex systems across natural sciences and engineering. However, directed graphs are trickier to work with as they cannot be represented as symmetric positive semi-definite matrices. Hence, Laplacian matrices for directed graphs may not be diagonalizable, and the eigenspaces of diagonalizable graphs may not exist in the real number space. Directed graphical models are ubiquitous in natural sciences and engineering as they can be used in modelling atomic structures to chemical reaction networks and neural systenms, Hence, developing a general graph theory for arbitrary graphs is an important research problem.

1 Introduction

The core idea of spectral graph theory is to define graphs as matrices, and extract information about the graph by analyzing the matrix eigenspaces. This approach has proven to be incredibly effective in studying complex systems across natural sciences and engineering. The general idea boils down to representing a complex system as a graph, computing and visualizing the principal eigenspaces to find any invariant properties of the system. One interesting analogy is the Fourier transform, which takes in a complex multi-modal signal and separates the individual modes, and hence allowing us to pick and study the most significant frequencies. However, the vast majority of spectral graph theory literature focuses on un-directed graphs, that are defined via symmetric and positive semi-definite Laplacian matrices that are diagonilazable. Since the eigenspaces always lie in the real number space, it makes it convenient to study systems that can be represented as un-directed graphs. Directed graphs on the other

hand, cannot be represented with symmetric positive definite matrices. Since various complex systems such as chemical reaction networks, social networks and the brain fundamentally assume a directed graph structure, it is an important research direction to develop graph theoretical methods for directed graphical systems. The goal of this project is to review the research results and directions in this domain.

2 Methods

This section will lay out the methods, and the associated literature for directed graph spectral methods that can be used to study chemical reaction networks. There are three main papers that will be discussed in more detail and the fourth paper is a paper that was recommended by the professor of this class. there is a final section which is a quick review of papers that were not the focus of this report. The papers that I go in detail as follows - (i) Markov Chain approach developed by Fan Chung (ii) Spectral Graph Theory for Laplacians with positive and negative complex values by Bauer (iii) Sparsification methods for efficient eigenvalue algorithms and (iv) Singular value decomposition, which is a different and less explored approach. This section will start with introducing the main ideas and results from these three approaches. The final part of this section will be concluded with a much shorter reviews that lays out other interesting work being performed in this research field.

2.1 Modelling Directed Graphs with Markov Chains (Chung)

This method treats graphs as Markov chains, where each edge is defined as a transition probability between vertices [Chu05]. It is an important approach because stochastic chemical reaction networks fundamentally assume a Markov chain structure. The main idea is that since a Markov chain matrix is diagonilazable, one can construct a Laplacian matrix from the eigenvectors of the Markov matrix.

Let G be a directed graph with edges $E(G)$ and vertices $V(G)$, the paper first defines the notion of a "walk" throughout the graph as we now have direction associated with each edge. A walk is defined as a vector of vertex indices

$$w = [v_1, v_2, \dots v_n]\,. \tag{1}$$

where, (v_{i-1}, v_i) is an edge. If d_v is the degree of a given vertex v, then the transition probablity is defined as

$$M(i,j) = \begin{bmatrix} 0 & A \\ A & 0 \end{bmatrix}$$

This implies that if a vertex is strongly connected, then there a higher probability for transition to this vertex. There can be other ways of defining the transition probability, but this way ensures that each matrix entries are positive and real values. Additionally, if the graphs are weighted, the degrees are normalized in the range $0, 1$, to mimick a probablilty value. Since this is a positive matrix, the authors argue that there exists a left eigenvector ϕ (that is a row vector) associated with the matrix M according to the Perron–Frobenius theorem.

$$\phi M = \rho\phi. \tag{2}$$

With these definitions, the (normalized) Laplacian matrix is computed as

$$L = I - \frac{\Phi^{-1/2} M \Phi^{1/2} + \Phi^{-1/2} M \Phi^{1/2}}{2}, \tag{3}$$

Where $\Phi = \text{diag}(\phi)$. Next, the paper defines the directed combinatorial Laplacian

$$L = \Phi - \frac{\Phi M - M^h \Phi}{2}. \tag{4}$$

where, M^h is the conjugate transpose of M. This formulation can also be used to compute the Rayleigh quotient. Next, the concept of *circulation* is introduced. We define a function $F(u, v)$ that assigns a positive number to each edge. A vertex u is said to be circular if

$$\sum_{u:u\to v} F(u, v) = \sum_{v:u\to v} F(v, u). \tag{5}$$

This means that if we start at an index u, we can circle back to u by traversing the graph edges. This introduces a new notion of "flow" that is more unique than un-directed graphs as we have have a direction associated with each edge. A directed graph is said to be *Eulerian* if it is fully connected, i.e, if we were start from one edge, we should be able to return to this edge after visiting every edge.

We now move on to defining the Cheeger inequalities for the Laplacian matrix. For a subset of vertices S in a directed graph G, We start with defining *Cheeger* constant (equivalent to the isoperimetric ratio for un-directed graphs)

$$h(G) = \inf_S \frac{F_\phi(\partial S)}{\min\left\{F_\phi(S), F_\phi(\bar{S})\right\}}. \tag{6}$$

Where $\bar{S} = V(G) \cap S$, and ∂S being the boundary of S. The Cheeger inequality is then defined as

$$2h(G) \geq \lambda \geq \frac{h(G)}{2}. \tag{7}$$

This paper also goes further to compute the bounds for the Cheeger constants and convergence rates for the Markov processes. The really interesting aspect of this approach is the similarity to the theory behind un-directed graphs. However, the main challenge with this approach is that the Laplacian matrix is limited to how we define the transition probability. Gleich [Gle06] extended this approach for the graph clustering problem, which is used in order to find vertex communities using graph cuts.

2.2 Directed Graph Laplacians with Positive and Negative Weights (Bauer)

In 2010, Frank Bauer [Bau12] released a big paper studying normalized graph Laplacians for directed graphs with positive and negative weights. This paper is particularly distinct from Fan Chung's ideas due to it not focusing on strongly connected graphs, or assuming real eigenvalues. Let $G = (V, E, w)$ be a weighted directed graph on n vertices where V, E and w are the vertices, edges and weights respectively. We should note that a connection and weights are not particularly equivalent. A graph can have a connection, but the weight can be zero. For example, in chemical reaction networks, there can be an edge between two species but the rate of change parameter (equivalent to weight) can change in time and sometimes be zero. The unique aspect about this work is that it defines graph transitions with complex valued functions. First, Bauer sets the notation for general directed graphs. Let G be a directed graph, and let C(V) be the space of complex valued functions on V, i.e transition from one vertex to another. and let $\Delta : C(V) \to C(V)$ be defined as an operator that computes the directed Laplacian as

$$\Delta v(i) = v(i) - \frac{1}{d_i^{in}} \sum_j w_{ij} v(j). \tag{8}$$

The Laplacian operator has always an eigenvector $\lambda_1 = 0$ and the corrosponding eigenvector is a constant vector. If we were to multiply all weights with a constant c, the spectrum of Δ will remain invariant. The bounds for these eigenvalues are

$$1 - r \leq \min_{i:\lambda_i \neq 0} Real(\lambda_i) \leq \frac{|V_R|}{n - m_0} \leq \max_{i:\lambda_i \neq 0} \leq 1 + r$$

where $r = \max(r_i)$, and $r_i = \frac{\sum_{j \in V} w_{ij}}{|d_i^{in}|}$, which is the radius of the complex plane where all the eigenvalues exist. m_i is the multiplicity of the eigenvalue i. Next, we look at the concept of *isolated vertices*. A vertex i is said to be isolated if $w_{ij} = 0 \forall j$.

The paper also defines quasi-isolated vertices which have the property

$$d_i^{in} = \sum_j w_{ij}. \tag{9}$$

where d_i^{in} represents the degree associated with all the edges that are pointing towards i. Next, we look at induced subgraphs for the directed graphs. Let G be a directed graph, a matrix G' is said to be an induced subgraph of G if

$$V' \subseteq V, \tag{10}$$

$$E' = E \cap (V'XV') \subseteq E \tag{11}$$

$$w' : V'XV' \to R \tag{12}$$

. The purpose of the induced subgraph is to find a matrix that excludes all of the isolated vertices, but retains all of the edges This definition makes sure we do not exclude quasi-isolated vertices. Now, consider a graph G and let $G_i, 1 \leq i \leq r$ be a subgraph only comprised of the strongly connected components then

- If G_i is isolated (i.e all the connected weights are equal to zero), then the Laplacian $L_G = 0 \forall j > 1$.
- If G_i is quasi-isolated then $\sum_{i=0}^{r} L_{j,i} = 0$.

Now we move on to Acyclic graphs, which are defined with the two following conditions - (i) all edges have the same direction and (ii) there are no cycles in the graph, meaning there is no path for a vertex that leads to itself. The Laplacian represented in Frobenius normal form is upper triangular, which implies that the nullspace of the Laplacian exists in $\{0, 1\}$. The extreme eigenvalues of a Laplacian are the ones that exist on the boundaries of the complex space (i.e $\lambda : |1 - \lambda| = r$). The paper then defines a graph G' to be a maximal *induced subgraph* of a acyclic directed graph G if all vertices $i \in V$ satisfy

$$r(i) = \max_i r(l) = r. \tag{13}$$

Where, r(i) represents the distance of the eigenvalue from the origin in the complex space.

The paper extends these ideas to other type of directed graphs such as k-partite graphs, anti k-partite graphs, bipartite graphs and compares the models in a rigorous manner. However, they were ommited from this report as the purpose it to introduce the main ideas.

2.3 Sparsification (Cohen et al)

This section covers the problem of developing efficient algorithms for computing Laplacian solvers for dense directed graphs via sparsification. The motivation for using sparsification is to convert an arbitrary directed graph into an Eulerian graph. The focus will mainly be on the work of Cohen et al [CKP+17], who developed algorithms based on efficient Laplacian solvers developed by Peng and Speilman [PS14]. The motivation for this is that it is much more efficient and stable to compute eigenspaces of sparse matrices. Their main achievement was to come up with an algorithm that runs in $\tilde{O}(nm^{\frac{1}{3}} + mn^{\frac{1}{3}})$. We first define matrix ϵ approximation for directed graphs (un-symmetric matrices). Let $U = \frac{1}{2}(L + L^t)$, then we define the matrix $\tilde{L}$ as an ϵ approximation of the Laplacian matrix L if it satisfies the following conditions [CKP+17].

- $\mathcal{N}(U) \in \mathcal{N}(\tilde{L} - L) \cap \mathcal{L}((\tilde{L} - L)^t)$.
- $||U^{\frac{-1}{2}}(\tilde{L} - L)U^{\frac{1}{2}}||$

Where, $\mathcal{L}(\cdot)$ represents the null space of a given matrix. The purpose of the null space restriction is to make sure that the optimization problem for computing the eigenspaces is bounded.

The next ingredient for the algorithm is *Eulerian scaling*. For a given directed graph Laplacian, there exists a vector x, such that $L \cdot diag(x)$ is an Eulerian matrix. We also consider the directed graph approximation. Next, for quantifying matrix similarity, we define the ϵ-approximation. Two Eulerian matrices $L \cdot \text{diag}(x)$ and $L \cdot \tilde{\text{diag}}(\tilde{x})$ are ϵ-approximate if

$$(1 - \epsilon)\,\text{diag}(x) <= \text{diag}(\tilde{x}) <= (1 + \epsilon)\,\text{diag}(x).$$

Once we determine the vector x, and the Laplacian matrix has been converted to an Eulerian matrix, the sparsification is done by the same algorithm as the one for undirected graphs. Next we move on to solving the linear system $Lx = b$. The first step is to decompose the matrix $L = D - A^t = D^{1/2}(I - \mathcal{A})D^{1/2}$, where $\mathcal{A} = D^{-1/2}A^tD^{1/2}$. The key idea of this paper is combine a technique called *square sparsifier chains* with the preconditioned Richardson iterative scheme. A square sparsifier chain is a series of matrix functions $\mathcal{A}_1, \mathcal{A}_2, \ldots \mathcal{A}_\lceil$ of length d with parameter 0 ¡ α ¡ 1/2 and error ϵ <= 1/2, and $L_i = I - \mathcal{A}_i$, and $A_i(\alpha) = +(1 - \alpha)\rangle \forall i$, the following conditions must be satisfied.

- $\mathcal{A}_i$ <= $1 \forall i$.
- $I - \mathcal{A}_i$ is an ϵ-approximation for $I - (\mathcal{A}(\alpha)_{i-1})^2$.

- $\mathcal{N}(L_i) = \mathcal{N}(L_i^t) = \mathcal{N}(U_{L_i}) \forall i.$

where U_{L_i} is the preconditioning matrix for L_i. The combination is done by inserting the preconditioned chains into the Richardson iteration step to approximate the matrix A. The runtime time for computing the sparsification chain of length d is $O(m + nd \exp O(\sqrt{dlog(d)}))$. And the runtime for the solver algorithm is $O(m + n2O(\sqrt{log(\kappa) * log(log(\kappa))})$, which is close to linear time.

2.4 Methods Based on The Singular Value Decomposition (Baglama et al.)

The singular value decomposition is an incredibly effective tool to study matrices. The SVD is defined as shown below

$$A = U\Sigma V^T = \sum_{j=1}^{n} \sigma_j u_j v_j. \tag{14}$$

Where Σ is a diagonal degree matrix holding the singular values, and the matrices U and V are orthogonal. By looking at the ordering of the singular values, one could pick the columns of U and V associated with the most significant and construct low-rank approximations of the matrix A, and it would be productive to look at the U, V matrices for directed graphs. This idea was first explored by Baglama et al [BFRR14], who proposed to use the partial SVD of the Laplacian to detect the most important nodes in a given graph. This paper was addressing some challenges associated with the paper by Benzi et al. [BEK13], who proposed to find the most significant nodes in a graph by analyzing the output of matrix functions such as the hyperbolic sine and cosine of the matrix

$$\mathcal{A} = \begin{bmatrix} 0 & A \\ A & 0 \end{bmatrix} \tag{15}$$

where A is the adjacency matrix of a directed graph. However, for large networks this approach can get intractable. Hence the authors propose the use of the singular value decomposition to reduce the computational cost. The authors idea is to instead of computing the matrix functions using the full adjacency matrix, construct a low-rank approximation of A by picking the top k significant singular values and the associated U and V vectors, and then apply the matrix functions to these reduced sub-spaces. If we apply the SVD to the function $exp(A)$, we get

$$\begin{bmatrix} \sqrt{AA^T} & As(\sqrt{AA^t}) \\ s(\sqrt{AA^t})A^t & \cosh\sqrt{A^TA} \end{bmatrix} \tag{16}$$

where,

$$s(x) = \begin{cases} x^{-1} sinh(x), & x \neq 0 \\ 1, & \text{otherwise} \end{cases} \tag{17}$$

This condition is to ensure that there is no zero division. We also define

$$As(\sqrt{AA^T} = A(\sqrt{AA^t})^{\dagger} sinh(\sqrt{AA^T}). \tag{18}$$

The SVD matrices hold key information of the range and null spaces of the corresponding full matrix. The Laplacian matrix of A is essentially a flow matrix that can be treated as a "walk" around the associated graph. Therefore the SVD matrices for the directed Laplacian is an interesting research direction. A null space would mean there is no movement in the graph and hence, these modes can be discarded. In this case, the matrices $\left[(AA^T)\right]$ and $\left[(A^TA)\right]$ correspond to the alternating walks. The original paper by Benzi uses the Gauss-type quadrature rules to determine upper and lower bounds of the form

$$u^T \exp(A)v, u, v \in R^{2n}. \tag{19}$$

To apply SVD to the form, simply plug in the block SVD form into the expression and simplifying.

$$A = \begin{bmatrix} U & 0 \\ 0 & V \end{bmatrix} \begin{bmatrix} 0 & \Sigma \\ \Sigma & 0 \end{bmatrix} \tag{20}$$

Where the blocks are singular values Σ, U and V matrices corresponding to the range and null spaces respectively. By doing this the authors were able to compute the bounds for the quadrature rules. The authors also talk about determining important nodes in a graph by looking at the singular values, i.e the nodes with the highest centrality's and the nodes with sparse connections, based on the Gaussian quadrature bounds. His main argument was to relate an undirected graph to a given directed graph.

2.5 Other Works

This section lays out some other methods for spectral graph theory for directed graphs. One of the earliest investigations for directed spectral graph theory was by Agev and Chebotarev where they study the spectra of directed graphs. They do this by looking at the characteristic polynomial of the adjacency matrices. They introduced the notion of a polygon shape associated with the Laplacian eigenvalues by proving that there exists a polygon shape where each point corresponds to an eigenvalue of the matrix associated with it. Steve Butler [But07], in his paper about relating the eigenvalues of a graphs G

and $G-H$, where H is a subgraph of G, he touches upon using this methods for directed graphs at the end of his paper. Chui et al [CMZ18] had a data science perspective for using directed graphs, where the authors developed a theory for representing functions for numerical data that can be represented as directed graphs (they use the simplified term digraphs). Their approach is to treat the digraph as a pair of undirected graphs, and look at the singular values of the two graphs. Their argument is that since we have a wealth of literature behind symmetric Laplacian matrices, it is worth it to define a directed graph as two un-directed graphs. Edinah and Murphy [GM20] developed a method for generalized estimation for the Rayleigh Quotient as most methods focus on Hermitian matrices. Fanuel et al [FAFS18] developed a method to visualize directed graphs by introducing the Magnetic Laplacian, which is a self-adjoint, positive semi-definite operator. They construct this matrix using the eigenspaces of the symmetric matrix $\frac{1}{2}(A + A^T)$ where A is the directed graph adjacency matrix.

3 Conclusions

This report reviews directed spectral graph theory methods methods that can be used to study chemical reaction networks, which fundamentally assume a directed graph structure. The further goal is to use these ideas in my own research of systems biology. Directed graphs are ubiquitous in nature and it is an important pursuit to investigate these structures in applied mathematics and computer science.

References

[Bau12] Frank Bauer. Normalized graph laplacians for directed graphs. *Linear Algebra and its Applications*, 436(11):4193–4222, 2012.

[BEK13] Michele Benzi, Ernesto Estrada, and Christine Klymko. Ranking hubs and authorities using matrix functions. *Linear Algebra and its Applications*, 438(5):2447–2474, 2013.

[BFRR14] J Baglama, Caterina Fenu, L Reichel, and Giuseppe Rodriguez. Analysis of directed networks via partial singular value decomposition and gauss quadrature. *Linear Algebra and its Applications*, 456:93–121, 2014.

[But07] Steve Butler. Interlacing for weighted graphs using the normalized laplacian. *The Electronic Journal of Linear Algebra*, 16:90–98, 2007.

[Chu05] Fan Chung. Laplacians and the cheeger inequality for directed graphs. *Annals of Combinatorics*, 9(1):1–19, 2005.

[CKP+17] Michael B Cohen, Jonathan Kelner, John Peebles, Richard Peng, Anup B Rao, Aaron Sidford, and Adrian Vladu. Almost-linear-time algorithms for markov chains and new spectral primitives for directed graphs. In *Proceedings of the 49th Annual ACM SIGACT Symposium on Theory of Computing*, pages 410–419, 2017.

[CMZ18] Charles K Chui, HN Mhaskar, and Xiaosheng Zhuang. Representation of functions on big data associated with directed graphs. *Applied and Computational Harmonic Analysis*, 44(1):165–188, 2018.

[FAFS18] Michaël Fanuel, Carlos M Alaíz, Ángela Fernández, and Johan AK Suykens. Magnetic eigenmaps for the visualization of directed networks. *Applied and Computational Harmonic Analysis*, 44(1):189–199, 2018.

[Gle06] David Gleich. Hierarchical directed spectral graph partitioning. *Information Networks*, 443, 2006.

[GM20] Edinah K Gnang and James M Murphy. Spectral analysis of non-hermitian matrices and directed graphs. *Linear Algebra and its Applications*, 604:72–91, 2020.

[PS14] Richard Peng and Daniel A Spielman. An efficient parallel solver for sdd linear systems. In *Proceedings of the forty-sixth annual ACM symposium on Theory of computing*, pages 333–342, 2014.