Fitting Regressions to Eigenvalues of Graphs

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Abstract

Spectral graph theory connects graph structure to the eigenvalues of its adjacency and Laplacian matrices. In this project, we analyze how these eigenvalues evolve as the number of vertices increases across various graph families. We validate known formulas for path and cycle graphs, then extend our analysis to k-regular, complete, and k-partite graphs. Using regression techniques, we approximate spectral values and explore new families such as tailed graphs, where we observe that the maximum Laplacian eigenvalue grows linearly with the number of tails. Our findings offer tools for fast approximation and applications in network science and chemistry, while suggesting future directions for formal proofs and bounded-error estimates.

Introduction and Literature Review

Spectral Graph Theory

Spectral graph theory is the study of the structural properties of graphs through the eigenvalues and eigenvectors of matrices associated with them, most notably the adjacency matrix and the Laplacian matrix. These spectral characteristics encode deep information about graph connectivity, expansion, and symmetry. In this project, we investigate how their spectral properties evolve as the number of vertices increases. Our primary goals are to:

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- Uncover relationships between the eigenvalues of adjacency and Laplacian matrices across various graph families,
- Analyze how these spectra evolve as the number of vertices increases, providing insight into the asymptotic behavior of large or growing graphs.

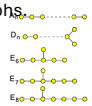

Figure 1: Example of Different Types of Graphs Explored[1]

Literature Review

We started our research by conducting a thorough literature review of the known relationships. Below are two graphs that we created illustrating the relationships $\lambda_k(L) = 2 + 2\cos\left(\frac{\pi k}{n}\right)$ for the Adjacency Matrix of a Path Graph and $\lambda_k(A) = 2\cos\left(\frac{\pi k}{n}\right)$ where n is the number of vertices and k is the index of the eigenvalue[2].

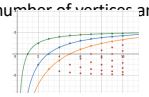

Figure 2: Eigenvalues of Adjacency

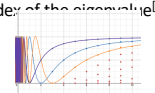

Figure 3: Eigenvalues of Laplacian

Useful Formulas

- **Perron Frobenius Theorem for Symmetric Matrices**[3]
  - Let G be a connected undirected graph with eigenvalues $\mu_1 \geq \mu_2 \geq \ldots \mu_n$
    - The eigenvalue μ_1 has a strictly positive eigenvector
    - $\mu_1 \geq -\mu_n$
    - $\mu_1 > \mu_2$
- **Max Eigenvalue Lemma**[3]
  - The maximum eigenvalue is bounded by the average degree and maximum degree of all vertices ($d_{ave} \leq \lambda_{max} \leq d_{max}$)

Our Work

Max Eigenvalue of k-Regular Graphs

A k-regular graph is a graph where all vertices have degree k, implying that the average degree equals the max degree. Using the lemma that the max eigenvalue is bounded by average/max degree, we found that for any k-regular graph $\boldsymbol{\lambda_{max} = k}$. This can be applied further to the following families:

Cycle Graphs: All vertices have degree 2, implying a max eigenvalue of 2 for any size cycle.

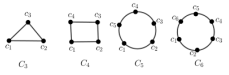

Figure 4: Cycle Graphs of size 3 to 6[6]

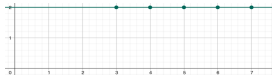

Figure 5: Eigenvalues of Cycles

Complete graphs: For a complete graph of size n, all vertices have degree n-1 implying a max eigenvalue of n-1

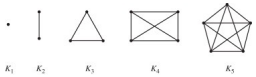

Figure 6: Complete Graphs of size 1 to 5[7]

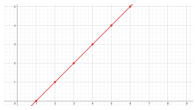

Figure 7: Max Eigenvalues of Complete graphs

K-Partite Complete Graphs: If we have a complete k-partite graph where all k-components have size n, then all vertices have degree and max eigenvalue n*(k-1)

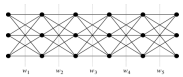

Figure 8: 5-Partite Complete Graph[8]

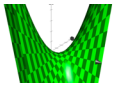

Figure 9: Max Eigenvalues of k-Partite Complete Graphs
(k on x-axis, n on y-axis: results in a parabolic surface)

Tailed Graphs

To explore how local structural changes affect spectral properties, we examine path graphs with increasing numbers of tail vertices attached to one end. These "tail-extended" graphs preserve the linear backbone of the path but introduce degree-1 vertices that alter the boundary conditions. As more tails are added, we observe notable changes in the Eigenvalues of both the Adjacency and Laplacian Matrices.

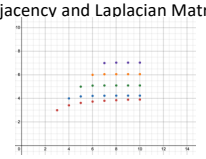

Figure 10: Eigenvalues of Laplacian for increasing tails.

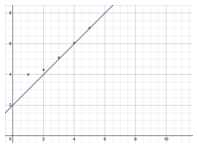

Figure 11: Bounds for Laplacian as tails increase

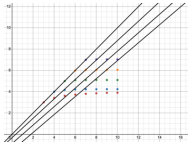

Figure 11: Linear Approximations

Figure 10 show the maximum eigenvalues of the Laplacian matrix as the number of vertices in the graph increases, color-coded by number of tails. We see that for each number of tails the maximum eigenvalue appears to approach an upper bound as the number of vertices increases. We plot this bound against number of tails in Figure 11 which demonstrates that the maximum eigenvalue seems to approach n+2 where n is the number of tails. Finally, in Figure 11 we estimate linear approximations for the maximum eigenvalue using number of tails as our independent variable for graphs with the same number of total vertices.

Conclusions and Next Steps

Our regression-based approach reveals consistent patterns in how graph structure influences spectral properties. By confirming known results and extending them to new families like tailed and k-partite graphs, we demonstrate that simple structural features can predict eigenvalue behavior with surprising accuracy.

Applications

1. **Fast Approximation**
   - Computing eigenvalues for large graphs can take $O(n^3)$ time, becoming extremely expensive for large graphs that model complex networks and datasets
   - Our regression would allow for a fast approximate solution, potentially in constant O(1) time, to this problem
2. **Epidemic Modelling**[4]
   - In certain models, the chance of an epidemic dying out in a network is bounded by $1/\lambda_{max}$ meaning that a larger max eigenvalue is correlated with a higher risk of outbreak
   - Thus we could model solutions to minimize the chances of a pandemic through removing nodes (vaccination), removing edges (quarantine communities), etc.
3. **Molecular Graphs for Chemistry**[5]
   - In chemistry, molecules can be modelled as graphs where vertices represent atoms and edges represent the chemical bonds between them
   - Eigenvalues correspond to molecular orbit, meaning the spectral gap between them can imply stability/instability

Next Steps

While our regression analysis provided us with estimations to the eigenvalues of these graphs, there is still a grey area on how effective our methods are. Firstly, we would hope to attempt to prove some of the relationships between the graphs and eigenvalues, such as seen in literature for cycle/path graphs. Finding an exact formula would be key to solving this problem. If unable to, we would then hope to understand how effective our analysis is in predicting these values by calculating an approximation factor to bound the effectiveness of our regression. This would be necessary so that anyone applying our approximate methods would be aware of possible errors in the calculation.

Acknowledgements

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