Heat Flow on a Graph

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1 Introduction

Heat flow on a weighted graph with N vertices is governed by the linear equation $\frac{dx}{dt} = Lx$, where x is an $N-$dimensional vector giving the temperatures at the vertices, and L is the Laplacian matrix for the weighted graph. If $x(t)$ is a solution to this equation, then

$$\lim_{t\to\infty} x(t) = \frac{1}{N}\sum_{i=1}^{N} x_i(0) \tag{1}$$

as long as L is negative semi-definite with a simple eigenvalue of 0. These conditions are satisfied for connected graphs with positive edge weights, for example. For a given graph G with variable edge weights and generic intial vertex temperatures, the convergence in (1) is fastest when the second largest eigenvalue of L (equivalently the largest nonzero eigenvalue) is minimum. Then to optimize the convergence in (1), it suffices to minimize the second largest eigenvalue of L by changing the edge weights. For a given graph G, let $\lambda_2(G)$ denote this minimum taken over all possible edge weight sequences γ subject to $\sum_{i=1}^{k}\gamma_i = 1$. In this paper, we numerically investigate some properties of the edges weights γ that achieve this minimum and the structure of the spectrum of the corresponding Laplacian for some example graphs. Finally, we make two conjectures that numerical test cases support: One, for an edge-transitive graph G, $\lambda_2(G)$ is achieved for uniform edge weights. Two, $\lambda_2(G)$ has multiplicity at least 2 for all connected G.

2 Non-Uniqueness of Minimizers

The first question we attempted to answer is whether $\lambda_2(G)$ is achieved by a unique minimizing sequence of edge weights γ. We quickly found numeric evidence to answer this question in the negative. An example is the complete bipartite graph $K_{2,4}$. Let $\gamma_1, \dots \gamma_4$ denote the weights of the 4 edges connecting the firxt top vertex to the 4 bottom vertices in this graph. Let $\gamma_5, \dots \gamma_8$ denote the weights of the other 4 edges containing the second top vertex. Then $\lambda_2(K_{2,4})$

is achieved when $\gamma_i = \begin{cases} \frac{1}{10} & i \in \{1, \dots 4\} \\ \frac{3}{20} & i \in \{5, \dots 8\} \end{cases}$, but also when $\gamma_i = \frac{1}{8}$. In both these cases, the minimum is $-\frac{1}{4}$.

3 Minimizers with Negative Edge Weights

For many classes of graphs (complete, cyclic, bipartite, etc.) we examined, the edge weights that minimized $\lambda_2(G)$ were nonnegative. This naturally raises the question of whether or not negative edge weights could be present in the minimizers of a graph. We find that, when the edges of a graph are concentrated in sections of the graph, which are connected by a less dense subset of edges, the minimizer includes negative edge weights. One simple example of this is in the graph with vertex set = $\{1, 2, 3, 4, 5, 6\}$ and edge set = $\{(1, 2), (1, 3), (2, 3), (3, 4), (4, 5), (4, 6), (5, 6)\}$, shown in Figure 1.

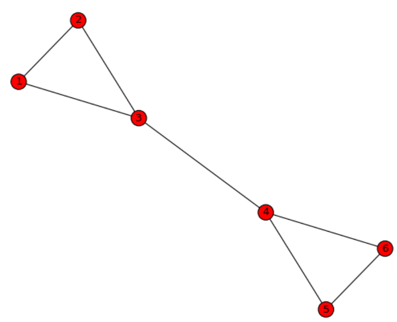

Figure 1: Graph G with $\lambda_2(G)$ achieved by edge weights of mixed sign

4 Graph Laplacians with Simple Eigenvalues

Initially, when exploring the sets of eigenvalues, we found no graph Laplacians with simple eigenvalues. Each set of eigenvalues had at least one eigenvalue of multiplicity ≥ 2. Furthermore, $\lambda_2(G)$ seems to always have multiplicity two. In a graph where the two largest nonzero eigenvalues may appear to be distinct, multiple evaluations of the program demonstrate that the difference between them becomes smaller as the prediction of $\lambda_2(G)$ becomes more accurate. This leads to a conjecture that $\lambda_2(G)$ always has multiplicity ≥ 2 for all connected graphs.

5 Edge- and Vertex-Transitive Graphs

A vertex-transitive graph is a graph where the automorphism group acts transitively on the vertices. An example is the truncated tetrahedron graph T, shown in Figure 2, which has 18 edges and 12 vertices.

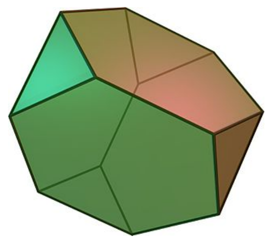

Figure 2: The truncated tetrahedron, T

Because of the symmetry of T, one might expect that the minimum of $\lambda_2(T)$ is achieved when $\gamma_i = \frac{1}{18}$ for all $i \in \{1, \ldots 18\}$. This expectation turns out to be false, however. Numerical evidence does show that this choice of γ_i is a critical point, but not a local minimum. Although T is vertex-transitive, it is not edge-transitive, which may explain this phenomenon.

In an edge-transitive graph, any edge can be mapped to any other edge by an automorphism. Certain graphs yield uniform minimizers. These include but are not limited to bipartite graphs, stars (which are simply a kind of bipartite graph of the form $K_{1,n}$), cycles, n-dimensional cubes, graphs representing platonic solids, complete graphs, and cycles. All of these graphs are edge-transitive, even though some are not vertex-transitive. An obvious example is that of the star graph From this a conjecture can be formed, namely that all edge-transitive graphs have uniform edge weights as a minimizer.

Many of these graphs also yield eigenvalues of a high multiplicity. For example, the bipartite graph $K_{m,n}$ have 0, $\frac{1}{n}+\frac{1}{m}$, $\frac{1}{n}$, and $\frac{1}{m}$, with multiplicities 1, 1, n-1, and $m-1$, respectively. The eigenvalues of complete graphs are 0 and $\frac{2}{n-1}$ with respective multiplicities of 1 and $n-1$. An interesting result involved cyclic graphs. Though having uniform minimizers, the eigenvalues at most had a multiplicity of 2, regardless the size of the edge. For cycles of odd length, the characteristic polynomial $C(\lambda)$, when divided by its constant can be expressed as a perfect square multiplied by λ. For example the characteristic polynomial of a cycle of length 7 is $\lambda(49\lambda^3 + 49\lambda^2 + 7\lambda + 1)^2$. For cycles of even length n, the characteristic polynomial is a perfect square polynomial multiplied by $\lambda(n\lambda + 4)$.

However, while it may be conjectured that the all edge-transitive graphs have uniform weights as minimizers, the converse is not necessarily true. Some examples of non-edge-transitive graphs include any wheel graph (comparable to pyramids with an n-sided polygon) and the Tutte graph, neither of which are edge-transitive nor vertex-transitive.