ON THE DIRECTIONAL DERIVATIVE OF KEMENY’S CONSTANT

CONNOR ALBRIGHT*, KIMBERLY P. HADAWAY †, ARI HOLCOMBE POMERANCE‡, JOEL JEFFRIES†, KATE J. LORENZEN§, AND ABIGAIL K. NIX¶

Abstract. In a connected graph, Kemeny’s constant gives the expected time of a random walk from an arbitrary vertex $x$ to reach a randomly-chosen vertex $y$. Because of this, Kemeny’s constant can be interpreted as a measure of how well a graph is connected. It is generally unknown how the addition or removal of edges affects Kemeny’s constant. Inspired by the directional derivative of the normalized Laplacian, we derive the directional derivative of Kemeny’s constant for several graph families. In addition, we find sharp bounds for the directional derivative of an eigenvalue of the normalized Laplacian and bounds for the directional derivative of Kemeny’s constant.

Key words. Kemeny’s constant, normalized Laplacian, directional derivative of eigenvalues.

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1. Introduction. A graph $G$ has a set of vertices $V(G)$ and a set of edges $E(G)$. An edge connecting vertices $x$ and $y$ is written $e = \{x, y\}$, and we say that $x$ and $y$ are adjacent if there exists an edge between them. We say that a graph is simple if it has no loops (an edge going from one vertex back to itself) and no more than one edge between any two vertices. For a vertex $x$, the neighbors of $x$ are the vertices adjacent to $x$, and the degree of $x$, denoted $d_x$, is the number of neighbors of $x$. A graph is connected if for any pair of vertices $x, y$, there exists a path, or a sequence of edges, from $x$ to $y$.

Consider a random walk on the vertices and edges of a simple connected graph $G$. We can think of this as someone walking along the edges of the graph. Our walker starts by occupying vertex $x$, and in the next step, the walker moves to one of the neighbors of $x$ at random with uniform probability of $\frac{1}{d_x}$. Note that this is a finite Markov chain, whose probability transition matrix is defined as $T = D^{-1}A$. Here, $D$ is the diagonal matrix containing the vertex degrees, and $A$ is the adjacency matrix of $G$. Since $G$ is connected, $D$ is invertible.

When analyzing Markov chains, or random walks on graphs, we can look at the long-term or the short-term behavior. The long-term behavior is found by taking repeated powers of $T$. For a general Markov chain which is irreducible and primitive, each row converges to the stationary vector $w$ of the chain. For more details, see [5]. This vector $w$ is also a left eigenvector of $T$ with the corresponding eigenvalue 1. The stationary vector can be interpreted as where a random walker is likely to be during a long random walk, and is independent of the starting vertex. The short-term behavior is described by the mean-first passage times. These indicate the expected time (or number of steps), starting at some vertex $x$, to reach some other vertex $y$, denoted $m_{x,y}$.

Kemeny’s constant, denoted $K(G)$, combines the mean-first passage times and the stationary vector of
a graph $G$. For a vertex $x$, the weighted average of the mean-first passage times from $x$ to each other vertex in the graph, where the weights are the corresponding entries of the stationary vector results in the following parameter,

$$K(G) = \sum_{y=1}^{n} m_{x,y} w_y.$$  

Surprisingly, $K$ is not dependent on the starting vertex $x$, hence the name Kemeny’s constant.

Kemeny’s constant has many useful interpretations, including the spread of infectious diseases (how quickly will a disease reach epidemic levels), molecular conformation dynamics (presence or absence of metastable sets), and urban road networks (how well connected a network is). In general, a lower Kemeny’s constant means that a graph is more connected, and a higher Kemeny’s constant means that a graph is less connected.

Figure 1: A barbell graph consists of two cliques connected by a path. Removing an edge within the clique will decrease Kemeny’s constant. This contradicts our intuition that removing edges will always make a graph less connected.

For these and other applications, a big question is: How do changes in the network lead to changes in Kemeny’s constant? Given the relation to connectivity, one might assume Kemeny’s constant must decrease as edges are added to a graph. However, contrary to this intuition, there are some graphs where the removal of an edge decreases Kemeny’s constant, and some graphs where the addition of an edge increases Kemeny’s constant (see Figure 1). An open problem is how the removal or addition of edges affects Kemeny’s constant. Breen and Kirkland in [3] looked at how small perturbations in the transitional probabilities related to changes in Kemeny’s constant. They were able to find a condition number which could serve as a confidence interval if the probabilities were calculated with raw data. They used the fundamental matrix of the perturbed transition matrix to find the size of the change. We also look at small changes to probabilities, but remain in the context of simple connected graphs.

In particular, we use the connection between Kemeny’s constant and the spectrum of the normalized Laplacian matrix to compute how Kemeny’s constant changes as small changes are made to a graph. The normalized Laplacian matrix of a graph is given by $\mathcal{L} = I - D^{-\frac{1}{2}} AD^{-\frac{1}{2}}$ where $A$ is the adjacency matrix and $D$ is the degree diagonal matrix. Note that the probability transition matrix $T$ is similar to $D^{-\frac{1}{2}} AD^{-\frac{1}{2}}$. Therefore, building off the connection Levene and Loizou made between Kemeny’s constant and the spectrum of $T$ in [6], Kemeny’s constant can be computed as

$$K(G) = \sum_{\lambda_T \neq 1} \frac{1}{1 - \lambda_T}$$

$$= \sum_{\lambda_T \neq 0} \frac{1}{\lambda_T}.$$
where each $\lambda_L$ is an eigenvalue of $L$.

Calculating Kemeny’s constant using the spectrum of graph matrices allow us to use existing tools of spectral graph theory. Recently, there have been developments in the directional derivative of the eigenvalues of graph matrices by Askoy, Purvine, and Young in [1]. They derived the directional derivative of eigenvalues with respect to a vertex $x$, where all edges containing $x$ had a parameter $t$ added to their current weight (here, we assume all unweighted edges have weight 1 and all non-edges have weight 0). This idea can be extended to any set of edges (or non-edges) of the graph.

This directional derivative can be interpreted as the effect of a slight change to an edge (or non-edge) weight on the eigenvalues of a graph matrix. Since Kemeny’s constant can be calculated by the eigenvalues of the normalized Laplacian, it follows that the directional derivative can be extended to Kemeny’s constant. In this paper, we give results on the directional derivative of eigenvalues of the normalized Laplacian and the directional derivative of Kemeny’s constant. We explicitly find these values for some families of graphs and establish bounds.

2. Directional Derivative of Eigenvalues. For a parameterized Hermitian matrix, the derivative of an eigenvalue is defined as follows.

**Definition 2.1.** Let $M(t)$ be a parameterized real-valued symmetric matrix, with parameterized eigenpair $(\lambda(t), v(t))$. The derivative of an eigenvalue of $M(t)$ is defined as

$$\frac{d\lambda}{dt}(t) = v^T(t) \frac{dM}{dt}(t)v(t),$$

where $\frac{dM}{dt}$ is an entry-wise derivative of $M(t)$.

Askoy et al. in [1] gave the directional derivative of eigenvalues of the adjacency, combinatorial Laplacian, and normalized Laplacian matrices. We will focus on the normalized Laplacian.

$$L(t) = \begin{bmatrix}
1 & \frac{-1}{2} & \frac{-1}{\sqrt{2(3+t)}} & 0 \\
\frac{-1}{2} & 1 & \frac{-1}{\sqrt{2(3+t)}} & 0 \\
\frac{-1}{\sqrt{2(3+t)}} & \frac{-1}{\sqrt{2(3+t)}} & 1 & \frac{-1-t}{\sqrt{(1+t)(3+t)}} \\
0 & 0 & \frac{-1-t}{\sqrt{(1+t)(3+t)}} & 1
\end{bmatrix}$$

Figure 2: The parameterized paw graph with $E_C = \{\{u_3, u_4\}\}$ (i.e. one changing edge), and the associated normalized Laplacian.

The parameterized normalized Laplacian is a matrix representation of a parameterized graph $G$, where the parameter $t$ represents some change to the weight of some collection of edges of the graph. An example of this parameterization is shown in Figure 2. The derivative can be interpreted as being calculated with respect to a set of changing edges, $E_C$, instead of with respect to the particular parameter $t$. In general, we are interested in this derivative when $t = 0$ since we are looking at small changes in the graph. For convenience, we will write $\frac{d\lambda}{dt}(0)$ as $\frac{d\lambda}{dt}L(0)$ as $L$, and eigenpair $(\lambda(0), v(0))$ as $(\lambda, v)$. Additionally, we will use $v_x$ to mean the $x$th component of $v$. 

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Lemma 2.2 (Aksoy et al. [1]). Let $E_C$ denote a set of edges of $G$. Let $\lambda$ be an eigenvalue of multiplicity $k$ for $L$ of $G$, and let $V = \{v_1, v_2, \ldots, v_k\}$ be an orthonormal basis for the eigenvectors associated with $\lambda$. Then,

\[
\frac{d\lambda}{dE_C} = \frac{1}{k} \sum_{i=1}^{k} \left[ (1 - \lambda) \sum_{\{x,y\} \in E_C} \left( \frac{\langle v_i \rangle x}{d_x} + \frac{\langle v_i \rangle y}{d_y} \right) - 2 \sum_{\{x,y\} \in E_C} \frac{\langle v_i \rangle x \cdot \langle v_i \rangle y}{\sqrt{d_x d_y}} \right].
\]

Observation 2.3. This derivative is linear in edges in $E_C$. Therefore, we consider the derivative of an eigenvalue with respect to a single edge knowing we can combine results to find the derivative with respect to any collection of edges.

The remainder of this section is organized as follows. Section 2.1 focuses on the directional derivative for particular graph structures. Section 2.2 establishes results for general graph families. Finally, we complete our analysis by examining results related to the directional derivative for non-edges in Section 2.3 and general bounds in Section 2.4.

2.1. Special Graph Structure. For any graph, the normalized Laplacian always has the eigenvalues $\lambda = 0$ and $\lambda = 2$, and these each have special meaning related to the graph. The eigenvalue $\lambda = 0$ is called the algebraic connectivity of the graph, since its multiplicity is the number of connected components of the graph. It has a well-known eigenvector, namely $D^\frac{1}{2} \mathbf{1}$.

Theorem 2.4. Let $G$ be a connected graph. Then, for the eigenvalue $\lambda = 0$ of $L_G$, the derivative $\frac{d\lambda}{d\{x,y\}}$ is zero with respect to any vertices $x, y$.

Proof. Let $G$ be a connected graph. Then, for $\lambda = 0$, it follows that $k = 1$. Let $x, y$ be any two vertices in $G$. Therefore,

\[
\frac{d\lambda}{d\{x,y\}} = \frac{\sqrt{d_x^2}}{d_x} + \frac{\sqrt{d_y^2}}{d_y} - 2 \frac{\sqrt{d_x} \sqrt{d_y}}{\sqrt{d_x d_y}}
= (1 + 1) - 2 \cdot 1
= 0.
\]

Note that the eigenvector does not need be normalized because the normalization scalar can be factored out of each sum, and the resulting value will still be 0.

Since the eigenvalue derivative is linear in edges, we have the following corollary.

Corollary 2.5. Let $E_C$ be a collection of edges of $G$. Then, $\frac{d\lambda}{dE_C} = 0$ for the eigenvalue $\lambda = 0$.

A graph has eigenvalue $\lambda = 2$ if and only if the graph is bipartite. Additionally, the multiplicity is the number of bipartite components of the graph. It also has a well-known eigenvector (for a connected graph). This allows us to establish the following results about the derivatives.

Theorem 2.6. Let $G$ be a connected bipartite graph. Then, for the eigenvalue $\lambda = 2$ of $L_G$, the derivative $\frac{d\lambda}{d\{x,y\}}$ is zero with respect to any edge $\{x, y\}$.

Proof. Let $G$ be a connected bipartite graph. The eigenvalue $\lambda = 2$ in $L$ has multiplicity $k = 1$ and corresponds to the eigenvector $v = D^\frac{1}{2} \begin{bmatrix} 1 \\ -1 \end{bmatrix}$. 

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Since $G$ is bipartite, we know that $x$ and $y$ are in different parts, and so $v_x$ and $v_y$ have opposite signs. Thus,

$$\frac{d\lambda}{d\{x, y\}} = (1 - 2) \left( \frac{v^2_x}{d_x} + \frac{v^2_y}{d_y} \right) - 2 \frac{v_x v_y}{\sqrt{d_x d_y}}$$

$$= -1 \left( \frac{(\pm \sqrt{d_x})^2}{d_x} + \frac{(\mp \sqrt{d_y})^2}{d_y} \right) - 2 \frac{(\pm \sqrt{d_x})(\mp \sqrt{d_y})}{\sqrt{d_x d_y}}$$

$$= -(1 + 1) - 2(-1)$$

$$= 0.$$ 

Here as well, the eigenvector does not need to be normalized because the normalization scalar can be factored out of each sum and the resulting value will still be 0.

For the normalized Laplacian, a bipartite graph’s spectrum is symmetric about 1. This means that, for a bipartite graph $G$, if $\lambda \in \text{Spec}_L(G)$, then $(2 - \lambda) \in \text{Spec}_L(G)$. The eigenvectors of these symmetric eigenvalues also come in pairs, and we show that the directional derivative follows suit.

**Theorem 2.7.** Let $G = (A, B)$ be a bipartite graph with eigenvalue $\lambda \in \text{Spec}_L(G)$. Then

$$\frac{d(2 - \lambda)}{d\{x, y\}} = -\frac{d\lambda}{d\{x, y\}}$$

for any edge $\{x, y\}$.

**Proof.** Let $v_1 = \begin{bmatrix} u \\ w \end{bmatrix}$ be an eigenvector for eigenvalue $\lambda_1$ of $L$ such that $u$ contains the entries corresponding to the vertices in part $A$ and $w$ contains the entries corresponding to the vertices in part $B$. Since the eigenvalues of the normalized Laplacian are symmetric about 1, it follows that $v_2 = \begin{bmatrix} u \\ -w \end{bmatrix}$ is an eigenvector for the eigenvalue $\lambda_2 = 2 - \lambda_1$ of $L$.

Consider the directional derivative of $\lambda_2$ with respect to $\{x, y\}$ where $x$ and $y$ are from different parts of the bipartite graph. We have

$$\frac{d\lambda_2}{d\{x, y\}} = \frac{1}{k} \sum_{i=1}^{k} \left[ (1 - \lambda_2) \left( \frac{u^2_{i,x}}{d_x} + \frac{(-w)^2_{i,y}}{d_y} \right) - 2 \frac{u_{i,x} (-w)_{i,y}}{\sqrt{d_x d_y}} \right]$$

$$= \frac{1}{k} \sum_{i=1}^{k} \left[ -(1 - \lambda_1) \left( \frac{u^2_{i,x}}{d_x} + \frac{w^2_{i,x}}{d_x} \right) + 2 \frac{u_{i,x} w_{i,y}}{\sqrt{d_x d_y}} \right]$$

$$= \frac{1}{k} \sum_{i=1}^{k} \left[ (1 - \lambda_1) \left( \frac{u^2_{i,x}}{d_x} + \frac{w^2_{i,x}}{d_x} \right) - 2 \frac{u_{i,x} w_{i,y}}{\sqrt{d_x d_y}} \right]$$

$$= -\frac{d\lambda_1}{d\{x, y\}}. \quad \Box$$

Another graph structure that relates to the structure of the eigenvectors is twin vertices. Two vertices $x$ and $y$ are said to be *twin vertices* if their neighborhoods are equal (apart from each other), i.e., if $N(x) \setminus \{y\} = N(y) \setminus \{x\}$. We say $x, y$ are *connected twins* if they are twin vertices that are adjacent. If a graph has twin
vertices \( x_1, x_2 \), then \([1, -1, 0, \ldots, 0]^T\) is an eigenvector for all symmetric graph matrices. Using this, we obtain the following results about the directional derivative of the spectrum of a graph with respect to the edge between connected twin vertices.

**Theorem 2.8.** Let \( G \) be a graph with connected twins \( x, y \) such that \(|N(x)| = |N(y)| = d\). Then, \( \lambda = \frac{d+1}{d} \in \text{Spec}_L(G) \), and \( \frac{d\lambda}{d\{x,y\}} \leq \frac{1}{k} \left( \frac{d^2}{d^2} \right) \), where \( k \) is the multiplicity of \( \lambda \).

**Proof.** Let \( G \) be a graph with connected twins \( x, y \) as described above. Consider a vector \( v \) where \( v_x = 1/\sqrt{2}, v_y = -1/\sqrt{2}, \) and \( v_i = 0 \) for all other vertices \( i \). By computation, \( v \) is an eigenvector for \( L(G) \) with eigenvalue \( d\lambda \).

First, suppose the multiplicity \( k \) of \( \lambda = \frac{d+1}{d} \) is 1 (so \( v \) is the only eigenvector). Then,

\[
\frac{d\lambda}{d\{x,y\}} = (1 - \lambda) \left( \frac{(1/\sqrt{2})^2}{d} + \frac{(-1/\sqrt{2})^2}{d} \right) = 2 \frac{(1/\sqrt{2})(-1/\sqrt{2})}{d} = \frac{d - 1}{d^2}.
\]

Now, let \( k > 1 \). Since \( v \) is a normalized vector, we can extend it to an orthonormal basis of the eigenspace corresponding to \( \lambda \), denoted \( \{v, w_1, \ldots, w_{k-1}\} \). Moreover, for any vector \( w_i \) in this basis, the \( x \)-th and \( y \)-th entries will be equal, since \( w_i \) is orthogonal to \( v \). So, \( w_{i,x} = w_{i,y} \) for all \( i \). Thus,

\[
\frac{d\lambda}{d\{x,y\}} = \frac{1}{k} \left[ \frac{d - 1}{d^2} + \sum_{i=1}^{k-1} \left( 1 - \frac{d + 1}{d} \right) \left( \frac{w_{i,x}^2}{d} + \frac{w_{i,y}^2}{d} \right) - 2 \frac{w_{i,x}w_{i,y}}{d} \right]
\]

\[
= \frac{1}{k} \left[ \frac{d - 1}{d^2} + \sum_{i=1}^{k-1} \left( - \frac{d + 1}{d} \right) \left( 2 \frac{w_{i,x}^2}{d} \right) \right]
\]

\[
\leq \frac{1}{k} \left( \frac{d - 1}{d^2} \right),
\]

since the degree and \( w_{i,x}^2 \) must always be positive. \( \square \)

This is maximized when \( d = 2 \) and \( k = 1 \) for a directional derivative of \( \frac{d\lambda}{d\{x,y\}} = 1/4 \). Interestingly, for graphs on a small number of vertices, this is the largest directional derivative value for a single edge. We explore more extremal values in Section 2.4.

**Corollary 2.9.** Let \( G \) be a graph with connected twins \( x, y \) such that \(|N(x)| = |N(y)| = d\). For all \( \lambda \in \text{Spec}_L(G) \), if \( \lambda \neq \frac{d+1}{d} \), then \( \frac{d\lambda}{d\{x,y\}} \leq 0 \).

**Proof.** Consider the set of orthonormal eigenvectors constructed in the proof of Theorem 2.8. It follows, for all eigenvalues associated with eigenvectors \( w \), that

\[
\frac{d\lambda}{d\{x,y\}} = \frac{1}{k} \left[ \sum_{i=1}^{k} (-\lambda) \left( \frac{w_{i,x}^2}{d} + \frac{w_{i,y}^2}{d} \right) - 2 \frac{w_{i,x}w_{i,y}}{d} \right]
\]

\[
= \frac{1}{k} \left[ \sum_{i=1}^{k} (-\lambda) \left( 2 \frac{w_{i,x}^2}{d} \right) \right]
\]

\[
\leq 0.
\]

\( \square \)
We now turn our attention away from particular edges and instead to the directional derivative with respect to all edges in the graph.

**Theorem 2.10.** Let \( \lambda \) be an eigenvalue of the normalized Laplacian \( \mathcal{L} \) for a graph \( G \). The sum of the derivatives of \( \lambda \) over all edges in \( G \) is zero.

**Proof.** Suppose the multiplicity of \( \lambda \) is 1. Let \( E \) be the set of edges in the graph, and let \( V \) be the set of vertices. Then the sum of \( \frac{d\lambda}{d\{x,y\}} \) over all edges is given by

\[
\sum_{\{x,y\} \in E} \frac{d\lambda}{d\{x,y\}} = \sum_{\{x,y\} \in E} \left[ (1 - \lambda) \left( \frac{v_x^2}{d_x} + \frac{v_y^2}{d_y} \right) - 2 \frac{v_x v_y}{\sqrt{d_x d_y}} \right]
\]

\[
= (1 - \lambda) \sum_{\{x,y\} \in E} \left( \frac{v_x^2}{d_x} + \frac{v_y^2}{d_y} \right) - 2 \sum_{\{x,y\} \in E} \frac{v_x v_y}{\sqrt{d_x d_y}}.
\]

In the first sum, \( v_x \) is counted \( d_x \) times for each vertex \( x \) in the graph. Thus,

\[
\sum_{\{x,y\} \in E} \frac{d\lambda}{d\{x,y\}} = (1 - \lambda) \sum_{x \in V} \left( \frac{v_x^2}{d_x} \right) - 2 \sum_{\{x,y\} \in E} \frac{v_x v_y}{\sqrt{d_x d_y}}
\]

\[
= (1 - \lambda) \sum_{x \in V} \left( v_x^2 \right) - 2 \sum_{\{x,y\} \in E} \frac{v_x v_y}{\sqrt{d_x d_y}}
\]

\[
= (1 - \lambda)(1) - 2 \sum_{\{x,y\} \in E} \frac{v_x v_y}{\sqrt{d_x d_y}}
\]

because \( v \) is an orthonormal eigenvector, so the squares of its entries sum to 1.

From the derivation of the normalized Laplacian eigenvalue derivative in [1], the remaining sum can be rewritten to get

\[
\sum_{\{x,y\} \in E} \frac{d\lambda}{d\{x,y\}} = (1 - \lambda)(1) - \left( D^{-\frac{1}{2}} v \right)^T A'(t) \left( D^{-\frac{1}{2}} v \right),
\]

where \( D \) is the degree matrix of \( G \) and \( A'(t) \) is the entry-wise derivative of the adjacency matrix evaluated at \( t \). Since all edges are parameterized, \( A' = A \).

Therefore,

\[
\sum_{\{x,y\} \in E} \frac{d\lambda}{d\{x,y\}} = (1 - \lambda) - v^T D^{-\frac{1}{2}} A D^{-\frac{1}{2}} v
\]

\[
= (1 - \lambda) - v^T (I - \mathcal{L}) v
\]

\[
= (1 - \lambda) - v^T v + v^T \mathcal{L} v
\]

\[
= (1 - \lambda) - (1 - \lambda) v^T v
\]

\[
= 0.
\]

Thus, we get that the sum of the derivatives of \( \lambda \) over all edges in \( G \) is zero. \( \Box \)

The directional derivative of an eigenvalue \( \lambda \) over all edges can be thought of as the effect of changing each edge by the same amount on \( \lambda \). Since the normalized Laplacian’s spectrum does not change by scaling the graph by a constant, our result is expected.
2.2. Families of Graphs. With these tools we can now find the directional derivatives for several families of graphs.

In order to analyze the eigenvalue derivatives of complete graphs, we first need to determine the form of the eigenvectors of this family of graphs.

**Proposition 2.11.** There exists an orthonormal basis of \( \mathbb{R}^n \) of the following form:

\[
\frac{1}{\sqrt{n}} \begin{bmatrix}
1 \\
1/\sqrt{2} \\
1 \\
1 \\
\vdots \\
1
\end{bmatrix}
\begin{bmatrix}
1 \\
1/\sqrt{2} \\
0 \\
-1/\sqrt{2} \\
-\sqrt{2}/n(n-2)
\end{bmatrix}
\begin{bmatrix}
(\sqrt{n-2)/2n} \\
(\sqrt{n-2)/2n} \\
0 \\
0 \\
\vdots
\end{bmatrix}
\begin{bmatrix}
0 \\
0 \\
* \\
* \\
* 
\end{bmatrix}
\]

where * denotes an undetermined entry.

**Proof.** Let \( v_1 = \frac{1}{\sqrt{n}} \mathbb{1} \) and \( v_2 = [1/\sqrt{2}, -1/\sqrt{2}, 0, \ldots, 0] \) (both of dimension \( n \)) which are both normalized and orthogonal to one another. Let \( w_1 \in \mathbb{R}^{n-2} \) be a scalar of the all ones vector. Therefore, we can extend \( w_1 \) to an orthonormal basis of \( \mathbb{R}^{n-2} \), namely

\( w_1, w_2, \ldots, w_{n-2} \).

Let \( v_i = [0, 0, w_{i-1}] \) for \( 3 \leq i \leq n-1 \). Therefore, \( v_3, \ldots, v_{n-1} \) are pairwise orthogonal, orthogonal to \( v_1 \) (since \( w_i \) is orthogonal to \( w_1 \)), orthogonal to \( v_2 \), and normalized. Let \( v_n = [a, a, b, \ldots, b] \) for some \( a, b \in \mathbb{R} \). Note that this vector is orthogonal to \( v_2, \ldots, v_{n-1} \) for any choice of \( a, b \).

In order for \( v_n \) to be orthogonal to \( v_1, a, b \) must satisfy

\[
2a + (n-2)b = 0.
\]

In order for it to be normalized, \( a, b \) must satisfy

\[
2a^2 + (n-2)b^2 = 1.
\]

This system has a solution of \( a = \sqrt{(n-2)/2n} \) and \( b = -\sqrt{2/n(n-2)} \).

Therefore, we have a full set of orthonormal eigenvectors where we know at least the first two entries of all the vectors.

This orthonormal basis is a set of eigenvectors for the complete graph \( K_n \) which we use to establish results about the directional derivative.

**Theorem 2.12.** Let \( G \) be a complete graph \( K_n \). For any eigenvalue \( \lambda \) of the normalized Laplacian, \( \frac{d\lambda}{de} = 0 \) with respect to any edge \( e \).

**Proof.** Consider \( K_n \) where \( \text{Spec}_L(K_n) = \{0, \frac{n-1}{n} \} \) for the normalized Laplacian. Without loss of generality, let \( e = \{1, 2\} \). For \( \lambda = 0 \), we have \( \frac{d\lambda}{de} = 0 \) by Theorem 2.4. Let \( \lambda = \frac{n-1}{n} \). By Proposition 2.11, we know the first two entries of an orthonormal set of eigenvectors for the eigenspace. Denote this set of vectors as \( \{v_2, \ldots, v_n\} \). Then,

\[
\frac{d\lambda}{de} = \frac{1}{n-1} \sum_{i=2}^{n} \left( 1 - \frac{n}{n-1} \right) \left( \frac{v_{i,1}^2}{d_1} + \frac{v_{i,2}^2}{d_2} \right) - 2 \frac{v_{i,1}v_{i,2}}{\sqrt{d_1d_2}}
\]
\[
\begin{align*}
&= \frac{1}{n-1} \left[ \left( \frac{-1}{n-1} \right) \left( \frac{1}{n-1} \right) + \frac{2}{2(n-1)} + \left( 1 - \frac{n}{n-1} \right) \left( \frac{2(n-2)}{2n(n-1)} \right) - \frac{2(n-2)}{2n(n-1)} \right] \\
&= \frac{1}{n-1} \left[ \frac{-1}{(n-1)^2} + \frac{n-1}{(n-1)^2} + \left( \frac{-n}{n-1} \right) \left( \frac{n-2}{n(n-1)} \right) \right] \\
&= \frac{1}{n-1} \left[ \frac{-1}{(n-1)^2} + \frac{n-1}{(n-1)^2} + \frac{-n+2}{n(n-1)} \right] \\
&= 0,
\end{align*}
\]
as desired. \qed

Since complete bipartite graphs have well-known eigenvectors, we can also completely classify the directional derivative of their eigenvalues.

**Theorem 2.13.** Let \( G \) be a complete bipartite graph. If \( \lambda \) is an eigenvalue of \( L_G \), then
\[
\frac{d\lambda}{d\{x,y\}} = 0
\]
with respect to any edge \( \{x,y\} \).

**Proof.** Consider \( K_{m,n} \), which has spectrum \( \text{Spec}_L(K_{m,n}) = \{0,1^{(m+n-2)},2\} \). For \( \lambda = 0 \) and \( \lambda = 2 \), \( \frac{d\lambda}{d\{x,y\}} = 0 \) by Theorems 2.4 and 2.6.

For \( \lambda = 1 \), an orthonormal basis for the associated eigenspace will have \( m-1 \) vectors with a 0 in the last \( n \) entries, and \( n-1 \) vectors with a 0 in the first \( m \) entries. Since each edge is between the two parts, either \( v_{i,x} \) or \( v_{i,y} \) will be zero. Therefore,
\[
\frac{d\lambda}{d\{x,y\}} = \frac{1}{m+n-2} \sum_{i=1}^{m+n-2} \left( (1-1) \left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right) - 2 \frac{v_{i,x} v_{i,y}}{\sqrt{d_x d_y}} \right) = 0.
\]
Thus, \( \frac{d\lambda}{d\{x,y\}} = 0 \) with respect to any changing edge in the graph. \qed

In addition to the complete bipartite graphs, we can completely classify the directional derivative of the eigenvalues of complete multipartite graphs in which all parts are of equal size.

**Theorem 2.14.** Let \( G \) be a complete multipartite graph \( K_{n,n,\ldots,n} \). If \( \lambda \) is an eigenvalue of \( L_G \), then
\[
\frac{d\lambda}{d\{x,y\}} = 0
\]
with respect to any edge \( \{x,y\} \).

**Proof.** Consider \( K_{n,n,\ldots,n} \), the complete multipartite graph with \( m \) parts each of size \( n \). This graph has spectrum \( \text{Spec}_L(K_{n,n,\ldots,n}) = \{0,1^{(m(n-1))},\frac{m}{m-1}^{(m-1)}\} \). Consider an edge \( \{x,y\} \).

First, let \( \lambda = 0 \). By Theorem 2.4, we have \( \frac{d\lambda}{d\{x,y\}} = 0 \).

Now, let \( \lambda = 1 \). We can choose an orthonormal basis where, for each vector, the only non-zero entries occur at indices that represent a single part of the graph. In other words, since each edge is between two parts, either \( v_{i,x} \) or \( v_{i,y} \) will be zero. Therefore,
\[
\frac{d\lambda}{d\{x,y\}} = \frac{1}{m(n-1)} \sum_{i=1}^{m(n-1)} \left( (1-1) \left[ \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right] - 2 \frac{v_{i,x} v_{i,y}}{\sqrt{d_x d_y}} \right) = 0.
\]
Finally, let $\lambda = \frac{m}{m-1}$. We can choose the orthonormal basis of the eigenspace to be $\{v_i \otimes (\frac{1}{n} \mathbb{1}_n) : 1 \leq i \leq m\}$ where $v_i$ comes from the orthonormal eigenspace of $K_m$ for the eigenvalue $\frac{m}{m-1}$ as given in Proposition 2.11. It can be shown that the tensor product of a set of orthonormal vectors with a scaled all ones vector is a set of orthonormal eigenvectors. Therefore,

$$
\frac{d\lambda}{d\{x, y\}} = \frac{1}{m-1} \sum_{i=1}^{m-1} \left[ \left( 1 - \frac{m}{m-1} \right) \left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right) - \frac{2v_{i,x}v_{i,y}}{\sqrt{d_xd_y}} \right]
$$

$$
= \frac{1}{m-1} \left[ \left( -\frac{1}{m-1} \right) \left( \frac{1}{m-1} \right) + \frac{m-2}{m(m-1)} \right] + \frac{1}{m-1} - \frac{(m-2)}{m(m-1)}
$$

which follows the proof given for Theorem 2.12.

In the previous proof, we used the tensor product of two vectors to get the eigenvectors of a graph for normalized Laplacian. The tensor product of two graphs (see Figure 3) is a graph operation whose resulting eigenvectors of the normalized Laplacian are the tensor product of the eigenvectors of the two smaller graphs.

![Figure 3: Two graphs $G$ and $H$ and their tensor product $G \times H$. The graph $G \times H$ is a Crown graph, or a complete bipartite graph minus a perfect matching.](image)

**Definition 2.15.** Let $G$ and $H$ be graphs. The tensor product of $G$ and $H$, denoted $G \times H$, is the graph on the vertices $V(G) \times V(H)$ with edge $(g, h) \sim (g', h')$ if and only if $g \sim g'$ in $G$ and $h \sim h'$ in $H$.

This normalized Laplacian matrix will be of the form

$$
L_{G\times H} = [(I - L_H) \otimes (L_G - I)] + I,
$$

for the tensor product. Let $(v, \lambda)$ be an eigenpair for $L_G$ and $(u, \mu)$ be an eigenpair for $L_H$. Then $(v \otimes u, \lambda + \mu - \lambda\mu)$ is an eigenpair for $L_{G\times H}$.

One family of graphs that can be defined using tensor products is the crown graphs, i.e. the complete bipartite graphs minus a matching.

**Theorem 2.16.** Let $G$ be a crown graph on $2n$ vertices, in other words $K_{n,n}$ minus a perfect matching. Therefore, $G = K_n \times K_2$. If $\lambda$ is an eigenvalue of $G$, then $\frac{d\lambda}{d\{x,y\}} = 0$ with respect to any edge $\{x, y\}$.

**Proof.** Since $G = K_n \times K_2$, it follows $\text{Spec}_\big(G\big) = \{0, \frac{n}{m-1}^{(n-1)}, \frac{n-2}{m-1}^{(n-1)}, 2\}$. By Theorems 2.4 and 2.6, we know if $\lambda = 0, 2$ we have our result.
Let \( \{x, y\} = \{(g, h), (g', h')\} \) and \( \lambda = \frac{n}{n-1} \). We can choose an orthonormal basis of this eigenspace to be \( \{v_i \otimes u : 1 \leq i \leq n\} \) where \( v_i \) comes from the orthonormal eigenspace for the complete graph given in Proposition 2.11 and \( u = \frac{1}{\sqrt{n}} \begin{bmatrix} 1 \\ 0 \end{bmatrix} \). It can be shown that the tensor product of a set of orthonormal vectors with a scalar of the all ones is also orthonormal. Therefore,

\[
\frac{d\lambda}{d\{g, h\}, (g', h')^T} = \frac{1}{n-1} \sum_{i=1}^{n-1} (1 - \lambda) \left[ \frac{(v_i, g' u_{i, h})^2}{d_g d_h} + \frac{(v_i, g' u_{i, h'})^2}{d_g d_{h'}} \right] - 2 \left[ \frac{v_i, g' u_{i, h} u_{i, h'}}{\sqrt{d_g d_h d_{g'} d_{h'}}} \right],
\]

since we know what \( u \) is and since the degree of all vertices in \( K_2 \) is 1. Since \( v_i \) is an eigenvector of \( K_n \) and \( d_g \) are the degrees in \( K_n \), it follows that

\[
\frac{d\lambda}{d\{g, h\}, (g', h')^T} = \frac{1}{2(n-1)} \left[ (1 - \frac{n}{n-1}) \left[ \frac{1}{n-1} + \frac{n-2}{n(n-1)} \right] + \frac{1}{n-1} - \frac{n-1}{n(n-1)} \right],
\]

which is the same as the proof of Theorem 2.12. It follows that \( \frac{d\lambda}{d\{x, y\}} = 0 \).

From Theorem 2.7, we know that the derivatives of eigenvalues of bipartite graphs are symmetric. Therefore, if \( \lambda = \frac{n-2}{n-1} \), then \( \frac{d\lambda}{d\{x, y\}} = 0 \). □

Cycle graphs, \( C_n \), also have predictable eigenvectors. Inspired by [8], we use the following set of orthonormal eigenvectors \( v_k, u_k \) which eigenvectors for \( \lambda_k = 1 - \cos(\frac{2\pi k}{n}) \) for \( 1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor \) for the normalized Laplacian of the cycle graph,

\[
v_k = c \begin{bmatrix} 1, & \cos \left( \frac{2\pi k}{n} \right), & \cos \left( \frac{3(2\pi k)}{n} \right), & \ldots, & \cos \left( \frac{(n-1)(2\pi k)}{n} \right) \end{bmatrix}^T,
\]

\[
u_k = c \begin{bmatrix} 0, & \sin \left( \frac{2\pi k}{n} \right), & \sin \left( \frac{3(2\pi k)}{n} \right), & \ldots, & \sin \left( \frac{(n-1)(2\pi k)}{n} \right) \end{bmatrix}^T
\]

for some scaling constant \( c \in \mathbb{R} \). We note that \( C_n \) also has eigenvalues \( \lambda = 0 \) and \( \lambda = 2 \) when \( n \) is even.

**Theorem 2.17.** Let \( G \) be a cycle graph. If \( \lambda \) is an eigenvalue of \( \mathcal{L}_G \), then \( \frac{d\lambda}{d\{x, y\}} = 0 \) with respect to any edge \( \{x, y\} \).

**Proof.** Every edge of a cycle graph is isomorphic. So, without loss of generality, let \( e = \{1, 2\} \). First, consider \( \lambda = 0 \) and, when \( n \) is even, also \( \lambda = 2 \). By Theorems 2.4 and 2.6, \( \frac{d\lambda}{dc} = 0 \).

Let \( \lambda = 1 - \cos(\frac{2\pi k}{n}) \) for some \( 1 \leq k \leq \left\lfloor \frac{n}{2} \right\rfloor - 1 \). For an arbitrary choice of \( k \), the two eigenvector entries will be \( v_{k,1} = c, v_{k,2} = c \cos(\frac{2\pi k}{n}) \), \( u_{k,1} = 0 \), and \( u_{k,2} = c \sin(\frac{2\pi k}{n}) \) for some constant \( c \in \mathbb{R} \). Therefore,

\[
\frac{d\lambda}{dc} = \frac{1}{2} \left[ (1 - \lambda) \left( \frac{v_{k,1}^2}{d_1} + \frac{v_{k,2}^2}{d_2} + \frac{u_{k,1}^2}{d_1} + \frac{u_{k,2}^2}{d_2} \right) - 2 \frac{v_{k,1} v_{k,2} u_{k,1} u_{k,2}}{\sqrt{d_1 d_2}} - 2 \frac{u_{k,1}^2 u_{k,2}^2}{\sqrt{d_1 d_2}} \right]
\]

\[
= \frac{1}{2} \left[ (1 - 1 + \cos(\frac{2\pi k}{n})) \left( \frac{c^2}{2} + \frac{c^2 \cos^2(\frac{2\pi k}{n})}{2} + \frac{c^2 \sin^2(\frac{2\pi k}{n})}{2} \right) - 2 \left( \frac{c^2 \cos(\frac{2\pi k}{n})}{2} \right) \right]
\]

\[
= \frac{c^2}{4} \left[ \cos \left( \frac{2\pi k}{n} \right) \left( 1 + \cos^2 \left( \frac{2\pi k}{n} \right) \right) + \sin^2 \left( \frac{2\pi k}{n} \right) - 2 \cos \left( \frac{2\pi k}{n} \right) \right]
\]

\[
= \frac{c^2}{4} \left[ 2 \cos \left( \frac{2\pi k}{n} \right) - 2 \cos \left( \frac{2\pi k}{n} \right) \right] = 0,
\]

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as desired.

Based on these examples, one might hypothesize that all the directional derivatives are zero. However, this is not the case. We have only examined graphs with highly symmetrical eigenvectors, so it is natural that all of these families have the directional derivatives of their entire spectra be zero.

2.3. Directional Derivative of Non-Edges. The interpretation (and formula) of the directional derivative is not constrained to edges. There are also meaningful results found by taking the derivative with respect to non-adjacent pairs of vertices, which we call non-edges. These derivatives tell us how the eigenvalues change when adding edges to the weighted graph, rather than just when changing the weights of current edges. We can also think of a non-edge as an edge of weight zero. We note that Theorem 2.4 about \( \lambda = 0 \) directly extends to non-edges.

For a bipartite graph, when \( \lambda = 2 \), the directional derivative now depends on whether the two vertices in the non-edge are from the same part or not (see Figure 4).

Figure 4: A bipartite graph. The pair \( \{x_1, x_2\} \) is a non-edge between two vertices in the same part and the pair \( \{x_2, y_2\} \) is a non-edge between two vertices in different parts. Therefore, for \( \lambda = 2 \), \( \frac{d\lambda}{d\{x_1,x_2\}} = -\frac{2}{3} \) while \( \frac{d\lambda}{d\{x_2,y_2\}} = 0. \)

**Theorem 2.18.** Let \( G \) be a connected bipartite graph and \( \{x, y\} \) be a non-edge between two vertices in different parts of the graph. Then, for \( \lambda = 2 \) of \( \mathcal{L}_G \), \( \frac{d\lambda}{d\{x,y\}} = 0. \)

**Proof.** This follows from the same argument used in the proof of Theorem 2.6.

**Theorem 2.19.** Let \( G \) be a connected bipartite and \( \{x, y\} \) be a non-edge between two vertices from the same part of the graph. Then, for \( \lambda = 2 \) of \( \mathcal{L}_G \), \( \frac{d\lambda}{d\{x,y\}} = \frac{-2}{|E|}. \)

**Proof.** Let \( \{x, y\} \) be a non-edge, where both \( x \) and \( y \) are in the same part of the bipartite graph. The normalized corresponding eigenvector is

\[
\mathbf{v} = \frac{1}{\sqrt{2|E|}} D^{\frac{1}{2}} \left[ \begin{array}{c} 1 \\ -1 \end{array} \right],
\]

where \( |E| \) is the number of edges in the graph. Now, both \( x \) and \( y \) are in the same part, so \( v_x \) and \( v_y \) have the same sign. Therefore,

\[
\frac{d\lambda}{d\{x,y\}} = (1 - 2) \left( \frac{v_x^2}{d_x} + \frac{v_y^2}{d_y} \right) - 2 \frac{v_x v_y}{\sqrt{d_x d_y}}
= \frac{1}{2|E|} \left[ -(1 + 1) - 2(1) \right]
= -\frac{2}{|E|}.
\]
Looking at the non-edge between isolated twin vertices, we establish similar results to those of connected twins.

**Theorem 2.20.** Let $G$ be a graph with non-adjacent twins $x$ and $y$ with $|N(x)| = |N(y)| = d$. Then, $\lambda = 1 \in \text{Spec}_L(G)$ and $\frac{d\lambda}{d\{x,y\}} \leq \frac{1}{kd}$, where $k$ is the multiplicity of $\lambda$. Furthermore, when $k = 1$, then $\frac{d\lambda}{d\{x,y\}} = \frac{1}{2}$.

**Proof.** Let $G$ be a graph with non-adjacent twins $x$ and $y$ as described above. Consider a vector $v$ where $v_x = 1/\sqrt{2}$, $v_y = -1/\sqrt{2}$, and $v_i = 0$ for all other vertices $i$. By computation, $v$ is an eigenvector for $L(G)$ with eigenvalue 1.

First, suppose $k = 1$. Then $v$ is the only eigenvector and

$$\frac{d\lambda}{d\{x,y\}} = (1 - \lambda) \left( \frac{v_x^2}{d} + \frac{v_y^2}{d} \right) - 2 \frac{v_x v_y}{\sqrt{d^2}}$$

$$= 0 + \frac{1}{d}$$

$$= \frac{1}{d}.$$

Now, let $k > 1$. Since $v$ is a normalized vector, we can extend it to an orthonormal basis of the eigenspace corresponding to $\lambda$ denoted $\{v, w_1, \ldots, w_{k-1}\}$. Moreover, for any vector $w_i$ in this basis, the $x$th and $y$th entries will be equal since $w_i$ is orthogonal to $v$. So $w_{i,x} = w_{i,y}$ for all $i$. Thus,

$$\frac{d\lambda}{d\{x,y\}} = \frac{1}{k} \left[ \frac{1}{d} + \sum_{i=1}^{k-1} (1 - \lambda) \left( \frac{w_{i,x}^2}{d} + \frac{w_{i,y}^2}{d} \right) - 2 \frac{w_{i,x} w_{i,y}}{d} \right]$$

$$= \frac{1}{k} \left[ \frac{1}{d} + \sum_{i=1}^{k-1} (0) - \left( \frac{2w_{1,x}^2}{d} \right) \right]$$

$$\leq \frac{1}{k} \left( \frac{1}{d} \right)$$

since the degree must always be positive.

The derivative of this particular eigenvalue resulting from isolated twins is maximized when $d = 1$ and $k = 1$ for a directional derivative of $\frac{d\lambda}{d\{x,y\}} = 1$. For any pair of vertices in graphs on a small number of vertices, this was the largest directional derivative we found.

**Corollary 2.21.** Let $G$ be a graph with isolated twins $x, y$ with $|N(x)| = |N(y)| = d$. For all $\lambda \in \text{Spec}_L(G)$, if $\lambda \neq 1$, then $\frac{d\lambda}{d\{x,y\}} \leq 0$.

**Proof.** Consider the set of orthonormal eigenvectors constructed in the proof of Theorem 2.20. It follows for all eigenvalues associated with eigenvectors $w$,

$$\frac{d\lambda}{d\{x,y\}} = \frac{1}{k} \left[ \sum_{i=1}^{k} (1 - \lambda) \left( \frac{w_{i,x}^2}{d} + \frac{w_{i,y}^2}{d} \right) - 2 \frac{w_{i,x} w_{i,y}}{d} \right]$$

$$= \frac{1}{k} \left[ \sum_{i=1}^{k} -\lambda \left( \frac{2w_{1,x}^2}{d} \right) \right]$$

$$\leq 0,$$

since $\lambda \geq 0$. □
The vertices in each part of $K_{m,n}$ are sets of isolated twins. So, the result of Theorem 2.19 is consistent with Theorem 2.20 and Corollary 2.21.

2.4. Bounds on Directional Derivative. Looking generally over all graphs with respect to any edge or non-edge, we establish both an upper and lower bound on the directional derivative.

**Theorem 2.22.** For a connected graph, the derivative of an eigenvalue of the normalized Laplacian $L$ with respect to an edge $\{x, y\}$ is bounded by

$$-\lambda \leq \frac{d\lambda}{d\{x, y\}} \leq 2 - \lambda.$$ 

Moreover, these are tight bounds.

**Proof.** We know from Formula 2.1 that the directional derivative is

$$\frac{d\lambda}{d\{x, y\}} = \frac{1}{k} \sum_{i=1}^{k} \left[ (1 - \lambda) \left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right) - 2 \frac{v_{i,x}v_{i,y}}{\sqrt{d_xd_y}} \right]$$

$$= \frac{1}{k} \sum_{i=1}^{k} \left[ \left( \frac{v_{i,x}}{\sqrt{d_x}} - \frac{v_{i,y}}{\sqrt{d_y}} \right)^2 - \lambda \left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right) \right].$$

Looking at this rewritten equation for $\frac{d\lambda}{d\{x, y\}}$, it is clear that the first term in the sum,

$$\left( \frac{v_{i,x}}{\sqrt{d_x}} - \frac{v_{i,y}}{\sqrt{d_y}} \right)^2,$$

is always nonnegative. We also know that $v_{i,x}$ and $v_{i,y}$ each come from an orthonormal eigenvector, so

$$\left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right)$$

is at most 1. Thus, if we are trying to minimize $\frac{d\lambda}{d\{x, y\}}$, we get that

$$\frac{d\lambda}{d\{x, y\}} = \frac{1}{k} \sum_{i=1}^{k} \left[ \left( \frac{v_{i,x}}{\sqrt{d_x}} - \frac{v_{i,y}}{\sqrt{d_y}} \right)^2 - \lambda \left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right) \right]$$

$$\geq \frac{1}{k} \sum_{i=1}^{k} [0 - \lambda]$$

$$= \left( \frac{1}{k} \cdot k \right)(-\lambda)$$

$$= -\lambda.$$

We can also find an upper bound for $\frac{d\lambda}{d\{x, y\}}$. We rewrite $\frac{d\lambda}{d\{x, y\}}$ as

$$\frac{d\lambda}{d\{x, y\}} = \frac{1}{k} \sum_{i=1}^{k} \left[ (2 - \lambda) \left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right) - \left( \frac{v_{i,x}}{\sqrt{d_x}} + \frac{v_{i,y}}{\sqrt{d_y}} \right)^2 \right].$$
To maximize this, because we know that
\[
\left( \frac{v_{i,x}}{\sqrt{d_x}} + \frac{v_{i,y}}{\sqrt{d_y}} \right)^2
\]
is always nonnegative, we can underestimate it as zero. Again, we have that \( v_{i,x} \) and \( v_{i,y} \) come from an orthonormal eigenvector, so the sum
\[
\left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right)
\]
is at most 1. Thus,
\[
\frac{d\lambda}{d\{x, y\}} = \frac{1}{k} \sum_{i=1}^{k} \left[ (2 - \lambda) \left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right) - \left( \frac{v_{i,x}}{\sqrt{d_x}} + \frac{v_{i,y}}{\sqrt{d_y}} \right)^2 \right]
\]
\[
\leq \frac{1}{k} \sum_{i=1}^{k} [(2 - \lambda) - 0]
\]
\[
= \left( \frac{1}{k} \cdot k \right) (2 - \lambda)
\]
\[
= 2 - \lambda.
\]

Putting these bounds together, we have
\[
-\lambda \leq \frac{d\lambda}{d\{x, y\}} \leq 2 - \lambda.
\]

Both of these bounds are tight. First, the lower bound is achieved when \( \lambda = 0 \) for any connected graph \( G \). The upper bound is achieved when \( \lambda = 2 \) for a bipartite graph. In both these cases, \( \frac{d\lambda}{de} = 0 \) for any edge \( e \) by Theorems 2.4 and 2.6.

The bounds are also tight when \( G \) has a pair of non-isolated twins:

![Figure 5: A graph G and Spec_L(G) = \{0, 1, \frac{3\pm\sqrt{5}}{2}\}. It has adjacent twins v1, v2 and non-adjacent twins v4, v5.](image)

**Example 2.23.** Consider the graph in Figure 5. First, observe that for this graph, the normalized Laplacian has eigenvalue \( \lambda = 1 \) with multiplicity 1. For the non-adjacent twin vertices (labeled \( v_4 \) and \( v_5 \) in the diagram), notice that both have degree 1. By Theorem 2.20, \( \frac{d\lambda}{d\{v_4, v_5\}} = \frac{1}{2} = 1 \). This is the upper bound for \( \frac{d\lambda}{d\{x, y\}} \) (as shown by Theorem 2.22) Therefore, this bound is indeed tight.
To show other results, we can compute the directional derivative of the graph’s spectrum with respect to each pair of vertices. The results are separated into edges and non-edges:

| (a) Edges  | \( \lambda \rightarrow \frac{5+\sqrt{5}}{4} \) | \( \frac{5-\sqrt{5}}{4} \) |
|------------|------------------------------------------|------------------|
| \( \{v_1, v_2\} \) | 0 | 0 | \(-0.07\) | \(-0.18\) |
| \( \{v_1, v_3\} \) | 0 | 0 | \(-\frac{1}{4}\) | \(-0.02\) | 0.15 |
| \( \{v_2, v_3\} \) | 0 | 0 | \(-\frac{1}{4}\) | \(-0.02\) | 0.15 |
| \( \{v_3, v_4\} \) | 0 | 0 | 0 | 0.06 | \(-0.06\) |
| \( \{v_3, v_5\} \) | 0 | 0 | 0 | 0.06 | \(-0.06\) |

| (b) Non-Edges | \( \lambda \rightarrow \frac{5+\sqrt{5}}{4} \) | \( \frac{5-\sqrt{5}}{4} \) |
|---------------|------------------------------------------|------------------|
| \( \{v_1, v_4\} \) | 0 | 0 | \(-\frac{1}{4}\) | \(-0.30\) | 0.43 |
| \( \{v_1, v_5\} \) | 0 | 0 | \(-\frac{1}{4}\) | \(-0.30\) | 0.43 |
| \( \{v_2, v_4\} \) | 0 | 0 | \(-\frac{1}{4}\) | \(-0.30\) | 0.43 |
| \( \{v_2, v_5\} \) | 0 | 0 | \(-\frac{1}{4}\) | \(-0.30\) | 0.43 |
| \( \{v_3, v_4\} \) | 0 | 1 | 0 | \(-0.72\) | \(-0.28\) |

Since \( v_1, v_2 \) are connected twins, for \( \lambda = \frac{3}{2} \), we have \( \frac{d\lambda}{d\{v_1, v_2\}} = \frac{1}{4} \), and, for \( \lambda \neq \frac{3}{2} \), we have \( \frac{d\lambda}{d\{v_1, v_2\}} \leq 0 \) by Theorem 2.8 and Corollary 2.9. Observe that for each eigenvalue in the edges table, the columns sum to zero (as shown by Theorem 2.10).

Not only is the bound tight for the graph given in the previous example, but for graphs on small \( n \), this type of structure gives the largest value of the directional derivative. This leads us to the following conjecture.

**Conjecture 2.24.** Over all graphs, the maximum directional derivative for any pair of vertices \( x, y \) is 1.

\[
\max_{G, \{x, y\}} \frac{d\lambda}{d\{x, y\}} = 1.
\]

**3. Directional Derivative of Kemeny’s Constant.** Using our formula for the directional derivative of the eigenvalue, we can also obtain a formula for the directional derivative of Kemeny’s constant. This derivative can be used to analyze how the value of Kemeny’s constant for a graph changes as one or some of its edge weights are changed. Since Kemeny’s constant is a measure of the connectivity of a graph, this derivative offers information about how changes in the graph structure affect connectivity.

Recall that Kemeny’s constant is calculated in terms of the eigenvalues of \( L \) by

\[
K(G) = \sum_{\lambda \neq 0} \frac{1}{\lambda}.
\]

As with the directional derivative of an eigenvalue, \( K \) can be differentiated with respect to a changing edge \( \{x, y\} \) in \( G \). Thus,

\[
\frac{dK}{d\{x, y\}} = \sum_{\lambda \neq 0} -\frac{1}{\lambda^2} \left( \frac{d\lambda}{d\{x, y\}} \right).
\]

Here, a positive value of \( \frac{dK}{d\{x, y\}} \) indicates that increasing the weight of edge \( \{x, y\} \) causes random walks between vertices to take longer and the graph to be less connected. On the other hand, a negative value of \( \frac{dK}{d\{x, y\}} \) indicates that increasing the weight of \( \{x, y\} \) causes random walks between vertices to get shorter and the graph to become more connected.

One might be tempted to assume that adding a non-edge to a graph always results in a negative value of \( \frac{dK}{d\{x, y\}} \) (and increases connectivity). This is not the case! Take, for example, an “almost” barbell graph,
i.e. a graph formed by taking a clique, a clique minus an edge, and connecting them with a path (see Figure 6). Taking the derivative of Kemeny’s constant with respect to the non-edge in the clique can in fact yield a positive value (less connected).

![Figure 6: An almost barbell becoming a true barbell](image)

Similar to the directional derivative of an eigenvalue, we can look at how Kemeny’s constant changes if we parameterize every edge.

**Theorem 3.1.** The directional derivative of Kemeny’s constant with respect to all edges in a graph $G$ sums to zero.

**Proof.** We begin by writing the sum of $\frac{dK}{dE}$ over all edges as

$$
\sum_{\{x,y\} \in E} \frac{dK}{d\{x,y\}} = \sum_{\{x,y\} \in E} \left( \sum_{\lambda \neq 0} \frac{d\lambda}{\lambda^2} \left( \frac{d\lambda}{d\{x,y\}} \right) \right).
$$

Switching the order of summation, we find

$$
\sum_{\{x,y\} \in E} \frac{dK}{d\{x,y\}} = \sum_{\lambda \neq 0} \left[ -\frac{1}{\lambda^2} \left( \sum_{\{x,y\} \in E} \frac{d\lambda}{d\{x,y\}} \right) \right].
$$

From Lemma 2.10, we know that $\sum_{\{x,y\} \in E} \frac{d\lambda}{d\{x,y\}} = 0$. Thus,

$$
\sum_{\{x,y\} \in E} \frac{dK}{d\{x,y\}} = \sum_{\lambda \neq 0} -\frac{1}{\lambda^2} \cdot 0 = 0.
$$

### 3.1. Families of Graphs.

As with the directional derivative of the eigenvalue, we can find results for the directional derivative of Kemeny’s constant for different families of graphs. The proofs for $\frac{dK}{d\{x,y\}}$ follow nicely and without difficulty from those for $\frac{d\lambda}{d\{x,y\}}$.

**Theorem 3.2.** Let $G$ be a complete graph $K_n$, a complete bipartite graph $K_{n,m}$, a complete multipartite graph $K_{n,n,...,n}$, a complete bipartite graph minus a matching, or a cycle graph $C_n$. Let $K$ be Kemeny’s constant for $G$ and $\{x,y\}$ be an edge of $G$. Then, $\frac{dK}{d\{x,y\}} = 0$.

**Proof.** By Theorems 2.12, 2.13, 2.14, 2.16, and 2.17, we have that $\frac{d\lambda}{d\{x,y\}} = 0$ for every eigenvalue $\lambda$ of $G$. Therefore,

$$
\frac{dK}{d\{x,y\}} = \sum_{\lambda \neq 0} -\frac{1}{\lambda^2} \left( \frac{d\lambda}{d\{x,y\}} \right) = \sum_{\lambda \neq 0} -\frac{1}{\lambda^2} \cdot 0 = 0,
$$
as desired.

3.2. Bounds and Extreme Values. Computing the directional derivative of Kemeny’s constant with respect to a changing edge allows us to determine exactly which edges in a graph have the greatest impact on overall graph connectivity when their weights are modified.

With this derivative explicitly defined, we can find the bounds on \( \frac{dK}{d\{x,y\}} \) for some edge (or non-edge) \( \{x,y\} \).

**Theorem 3.3.** The directional derivative of Kemeny’s constant \( \frac{dK}{d\{x,y\}} \), is bounded as follows:

\[
\sum_{\lambda \neq 0} \left( \frac{-2}{\lambda^2} \right) + K \leq \frac{dK}{d\{x,y\}} \leq K.
\]

**Proof.** We can easily find these bounds by substituting our bounds for \( \frac{d\lambda}{d\{x,y\}} \), found in Theorem 2.22, into the formula for \( \frac{dK}{d\{x,y\}} \). Doing this for both the upper and lower bounds of \( \frac{dK}{d\{x,y\}} \), we get that

\[
\sum_{\lambda \neq 0} \frac{-1}{\lambda^2} (2 - \lambda) \leq \frac{dK}{d\{x,y\}} \leq \sum_{\lambda \neq 0} \frac{-1}{\lambda^2} (-\lambda)
\]

\[
\sum_{\lambda \neq 0} \frac{-2}{\lambda^2} + \sum_{\lambda \neq 0} \frac{\lambda}{\lambda^2} \leq \frac{dK}{d\{x,y\}} \leq \sum_{\lambda \neq 0} \frac{\lambda}{\lambda^2}
\]

\[
\sum_{\lambda \neq 0} \frac{-2}{\lambda^2} + \sum_{\lambda \neq 0} \frac{1}{\lambda} \leq \frac{dK}{d\{x,y\}} \leq \sum_{\lambda \neq 0} \frac{1}{\lambda}
\]

Recall that Kemeny’s constant is found by \( K = \sum_{\lambda \neq 0} \frac{1}{\lambda} \). Thus, we have the bounds

\[
\sum_{\lambda \neq 0} \left( \frac{-2}{\lambda^2} \right) + K \leq \frac{dK}{d\{x,y\}} \leq K.
\]

Despite the bound for the directional derivative of eigenvalue being tight for certain graphs, it is unknown if either bound for the directional derivative of Kemeny’s constant is tight. Instead, we present two families of graphs that have the highest and lowest directional derivatives of Kemeny’s constant for graphs on up to 7 vertices and compare these values to the respective bounds.

**Figure 7:** The lollipop graph \( L_{3,n-3} \) with far edge \( \{n-1,n\} \)

**Maximum Value (Lollipop Graphs).** For graphs on \( n \leq 7 \) vertices, the maximum value of the derivative of Kemeny’s constant occurs on the lollipop graph consisting of a complete graph \( K_3 \) attached by
a bridge to a path graph on \( n - 3 \) vertices (see Figure 7) with respect to the edge at the far end of the path (i.e., the edge with greatest distance from the \( K_3 \) clique).

| \( n \) | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
|-------|---|---|---|---|---|----|----|----|
| Graph | \( L_{3,2} \) | \( L_{3,3} \) | \( L_{3,4} \) | \( L_{4,4} \) | \( L_{4,5} \) | \( L_{5,5} \) | \( L_{5,6} \) | \( L_{5,7} \) |
| \( \frac{dK}{d_{\{n-1,n\}}} \) | 1.06 | 1.86 | 2.58 | 3.51 | 4.38 | 5.28 | 6.28 | 7.22 |
| Upper Bound | 4.9 | 8.1 | 12.1 | 15.0 | 20.8 | 23.8 | 31.5 | 40.1 |

Table 1: The maximum directional derivative of \( K \) among lollipop graphs on \( n \) vertices with respect to the far edge, as well as the upper bound for that graph as generated by Theorem 3.2

One interpretation for this graph and edge giving a large value for the directional derivative of \( K \) comes from the characteristics of the barbell graph (see Figure 1). It is established that the barbell graph has the highest order of Kemeny’s constant at \( O(n^3) \) (see [2]). This high value for \( K \) is understood as a result of the two cliques acting as a sink in a random walk, increasing the mean first passage time.

The high value for the directional derivative of \( K \) on the lollipop graph can be interpreted similarly. By increasing the weight of the end of the path, the graph is in a way “barbellized”, where the far edge serves the same purpose as a clique in the barbell graph.

In general, the lollipop graph \( L_{r,s} \) refers to a complete graph \( K_r \) connected to a path graph on \( s \) vertices by a bridge. Table 1 lists the lollipop graph on \( n \) vertices (for \( 5 \leq n \leq 12 \)) that yields the highest directional derivative of \( K \) with respect to its far edge (labeled \( \{n-1,n\} \)), the computed value for this derivative, and the upper bound generated by Theorem 3.2.

The general extremal graph for the upper bound of the directional derivative of Kemeny’s constant is likely to be related to the lollipop graph. As seen in Table 1, the value of \( \frac{dK}{d_{\{n-1,n\}}} \) with respect to the far edge of the lollipop grows linearly, which is far from the cubic growth of the upper bound given by Theorem 3.2. This leads us to the following conjecture.

**Conjecture 3.4.** For a given \( n \), the directional derivative of Kemeny’s constant on simple graphs of order \( n \) is largest on a lollipop graph on \( n \) vertices with respect to the far edge. The value of this derivative grows \( O(n) \).

![Figure 8: Adding a non-edge to turn a path on \( n \) vertices into a cycle](image)

**Minimum Value (Path to Cycle).** For graphs on \( n \leq 7 \) vertices, the minimum value of the directional derivative of Kemeny’s constant occurs on the path graph with respect to the *non-edge* that forms a cycle graph when added (see Figure 8). Especially for larger values of \( n \), adding this edge has a dramatic effect on Kemeny’s constant, as shown in Table 2. Compared to the maximal value, this derivative’s magnitude is much larger.

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Table 2: The directional derivative of $K$ with respect to the path-to-cycle non-edge on $n$ vertices, as well as the lower bound for that graph as generated by Theorem 3.2

| $n$ | 5  | 6  | 7  | 8  | 9  | 10 | 11 | 12 |
|-----|----|----|----|----|----|----|----|----|
| $\frac{dK}{d(n,1)}$ | -9.4 | -19.2 | -34.0 | -54.9 | -82.7 | -118.5 | -163.4 | -218.2 |
| Lower Bound | -21 | -52 | -111.2 | -208 | -357 | -574.2 | -877.8 | -1288 |

4. Future Directions. In this paper, we provided bounds for the directional derivative of eigenvalues of the normalized Laplacian (Theorem 2.22) and for the directional derivative of Kemeny’s constant (Theorem 3.2). However, as the empirical data and our Conjectures 2.24, 3.4, and 3.5 suggest, these bounds can probably be improved. In particular, the current bounds give Kemeny’s constant bounded above by $O(n^3)$ and below by $O(n^6)$, but empirical data suggests that more appropriate bounds are above by $O(n)$ and below by $O(n^3)$.

Additionally, our focus was on unweighted, undirected graphs. Future work includes extending results to weighted derivatives. Instead of parameterizing the graph by $t$, the each parameterised edge $\{x, y\}$ would have value $w_{x,y}(1+t)$. The equation for the directional derivative of an eigenvalue of the normalized Laplacian would then become

$$\frac{d\lambda}{dE_C} = \frac{1}{k} \sum_{i=1}^{k} \left( (1 - \lambda) \sum_{\{x,y\} \in E_C} w_{x,y} \left( \frac{v_{i,x}^2}{d_x} + \frac{v_{i,y}^2}{d_y} \right) - 2 \sum_{\{x,y\} \in E_C} \frac{w_{x,y}v_{i,x}v_{i,y}}{\sqrt{d_xd_y}} \right).$$

If all the parameterizing weights are the same, then this has no effect. It is straightforward to compute that Theorems 2.4 and 2.6 stay consistent in this extension.

Extending results to directed graphs is more challenging. This is because the definition of the derivative of a matrix-eigenvector equation is only defined for Hermitian matrices. In the case of real-valued graph matrices, this constrains us to symmetric matrices. The normalized Laplacian has many spectral similarities to the probability transition matrix $D^{-1}A$, which is not symmetric. If $L\mathbf{v} = \lambda \mathbf{v}$ and $\mathbf{u} = D^{-1/2}\mathbf{v}$, then $D^{-1}A\mathbf{u} = (1 - \lambda)\mathbf{u}$. For a connected graph, the directional derivative of the eigenvalues, $\mu$, of the probability
transition matrix would be as follows,

$$\frac{d\mu}{EC} = \frac{1}{k} \sum_{i=1}^{k} \left[ \mu \sum_{(x,y) \in EC} \left( u_{i,x}^2 + u_{i,y}^2 \right) - 2 \sum_{(x,y) \in EC} u_{i,x} u_{i,y} \right].$$

This could be modified to include accommodate directed graphs as follows,

$$\frac{d\mu}{EC} = \frac{1}{k} \sum_{i=1}^{k} \left[ \mu \sum_{(x,y) \in EC} u_{i,x}^2 - \sum_{(x,y) \in EC} u_{i,x} u_{i,y} \right].$$

These results would further expand our knowledge of how small changes to directed and weighted graphs effect Kemeny’s constant.

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