Extremal graphs with minimal k-th Laplacian eigenvalue

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joint work with

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Graph Laplacian

The **graph Laplacian** of a simple graph $G = (V, E)$ with weights w_{uv} is defined by

$$\boxed{L(G) = D(G) - A(G)}$$

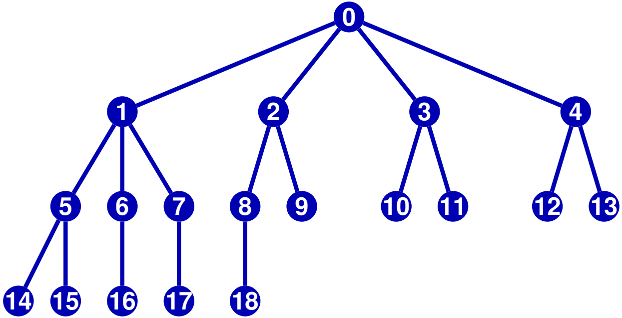
$A(G)$ ... adjacency matrix of G

$D(G)$ ... degree matrix with $D_{vv} = \sum_{u \sim v} w_{uv}$

with eigenvalues $0 = \lambda_1 \leq \lambda_2 < \cdots < \lambda_n$.

Extremal Graphs

Let $\mathcal{T}_\pi$ the class of all trees with prescribed degree sequence π. Then a tree T has maximal Laplacian spectral radius in $\mathcal{T}_\pi$ if and only if it can be constructed by breadth-first search. [Zhang, 2008]



Tree with degree sequence $\pi = (4^2, 3^4, 2^3, 1^{10})$

Rayleigh Quotient

Sketch of Proof:

1. **Rayleigh-Ritz Theorem:**

   λ_1 minimizes Rayleigh quotient

$$\mathcal{R}_L(f) = \frac{\langle f, Lf \rangle}{\langle f, f \rangle} = \frac{\sum_{uv \in E} w_{uv} (f(u) - f(v))^2}{\sum_{v \in V} f(v)^2}$$

   that is

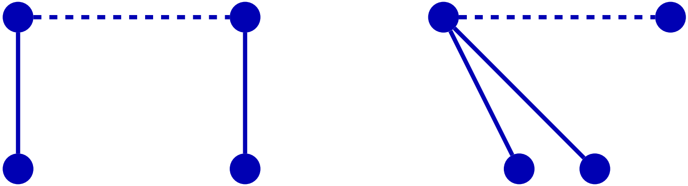
$$\lambda_1 = \min_{f \neq 0} \mathcal{R}_L(f)$$

   Function f that minimizes $\mathcal{R}_L(f)$ is eigenfunction.
   It can be assumed to be strictly positive (Perron vector).

Switching and Shifting

2. Rearrangement of edges:

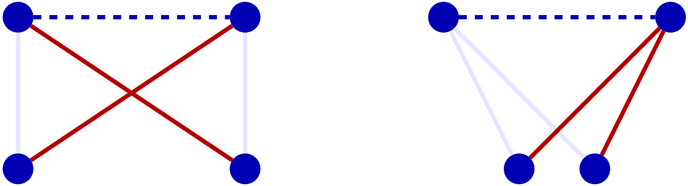
- Start with some graph G and eigenfunction (Perron vector) f.



Switching and Shifting

2. Rearrangement of edges:

- Start with some graph G and eigenfunction (Perron vector) f.
- Rearrange edges such that new graph G' belongs to same class.
- Compare Rayleigh quotients of f on these two graphs.



k-th Eigenvalue

Can this idea be used to characterize graphs that have miminal *k*-th eigenvalue among all graphs in the given class?

Problem: Have to use Courant-Fischer Theorem

$$\lambda_k = \min_{\substack{f \neq 0 \\ f \perp f_i \\ i = 1, \dots, k-1}} \mathcal{R}_L(f)$$

where f_i are eigenfunctions corresponding to the i-th eigenvalue.

Eigenfunction f_i on G need not be eigenfunction on G'.

That is, we have constraints for minimization problem that are hard to control.

Graph with Boundary

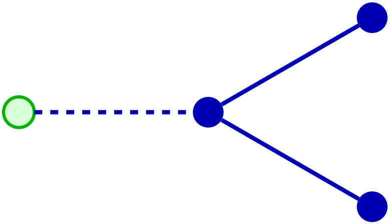
A **graph with boundary** is a graph $G^\circ = (V^\circ \cup \partial V, E^\circ \cup \partial E)$ where

V° ... interior vertices

∂V ... boundary vertices

E° ... interior edges $\subseteq V^\circ \times V^\circ$

∂E ... boundary edges $\subseteq V^\circ \times \partial V$



Dirichlet Matrix

The **Dirichlet matrix** is the graph Laplacian restricted to the interior vertices of a graph with boundary:

$$L^\circ(G) = D^\circ(G) - A^\circ(G)$$

$A^\circ(G)$ ... adjacency matrix of graph induced by V°
$D^\circ(G)$ ... degree matrix $D(G)$ restricted to V°

Hence $L^\circ(G)$ is the Laplacian $L(G)$ restricted to V°.

We denote the first Dirichlet eigenvalue by $\nu(G)$.

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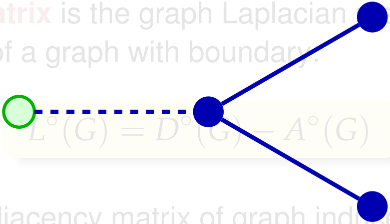

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$$L\ (T) = \begin{pmatrix} 1 & -1 & 0 & 0 \\ -1 & 3 & -1 & -1 \\ 0 & -1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$$

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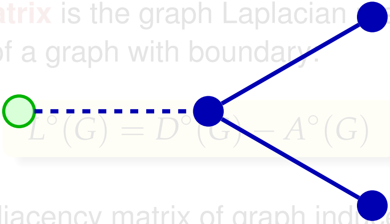

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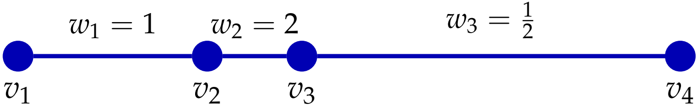
$$L^\circ(T) = \begin{pmatrix} 3 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

Geometric Realization

The **geometric realization** $\mathcal{G}$ of a graph G with weights w_{uv} is a metric space where the vertices are points and the edges uv correspond to arcs of length $1/w_{uv}$ that connects the incident vertices u and v.



Define two measures

$$\mu_V(\mathcal{G}) = |V| \qquad \ldots \text{ number of vertices}$$

$$\mu_E(\mathcal{G}) = \sum_{uv \in E} \frac{1}{w_{uv}} \qquad \ldots \text{ cumulated length of edges}$$

(Lebesgue measure on $\mathcal{G}$)

Rayleigh Quotient

For a vector f on G:

$$\mathcal{R}_L(f) = \frac{\langle f, Lf \rangle}{\langle f, f \rangle} = \frac{\sum_{uv\in E} w_{uv}(f(u) - f(v))^2}{\sum_{v\in V} f(v)^2}$$

For a continuous piecewise differentiable function ϕ on $\mathcal{G}$:

$$\mathcal{R}_{\mathcal{L}}(\phi) = \frac{\int_{\mathcal{G}} |\nabla \phi|^2 \, d\mu_E}{\int_{\mathcal{G}} |\phi|^2 \, d\mu_V}$$

The latter defines a continuous version of the graph Laplacian on $\mathcal{G}$: **geometric Laplacian $\mathcal{L}$**

The Geometric Laplacian

The eigenvalues of the geometric Laplacian $\mathcal{L}$ and the graph Laplacian G coincide.

The eigenfunctions of $\mathcal{L}$ are piecewise linear (on the edges of E). Their restrictions to V are exactly the eigenvectors of G.

[Friedman, 1993]

Nodal Domains

Let f be an eigenvector of G. We call the components of the two graphs induced by the vertices of non-negative and non-positive valuations the (strong) **nodal domains** of f.

(Perron components)

$$G[\{v : f(v) > 0\}] \qquad \text{and} \qquad G[\{v : f(v) < 0\}]$$

Geometric Nodal Domains

Let ϕ be the eigenfunction on $\mathcal{G}$ corresponding to eigenvector f on G.

- Insert new vertices where ϕ changes sign on an edge xy (and thus subdivide edges).
- Use arc lengths $\frac{|\phi(x)|}{|\phi(x)-\phi(y)|}$ and $\frac{|\phi(y)|}{|\phi(x)-\phi(y)|}$, resp.
  ϕ is eigenfunction of the new graph with same eigenvalue.
- All vertices where ϕ vanishes but have non-vanishing neighbors are considered as boundary vertices.
- Split all boundary vertices such that each component has vertices with non-zero valuation (all of same sign).

We call these components the **geometric nodal domains** of f.

Geometric Nodal Domains

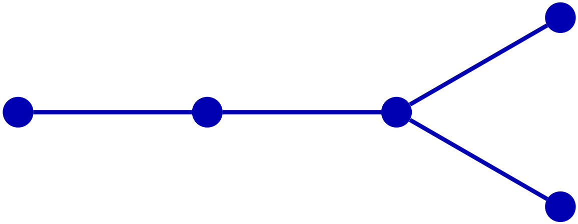
Let f be an eigenvector of G corresponding to eigenvalue λ.

The first Dirichlet eigenvalue at each of these geometric nodal domains coincides with λ.

f restricted to a geometric nodal domain is an eigenvector to the first Dirichlet eigenvalue [Bıyıkoğlu et al., 2007].

(This idea is related to the bottleneck matrix introduced in [Kirkland et al., 1996].)

Example



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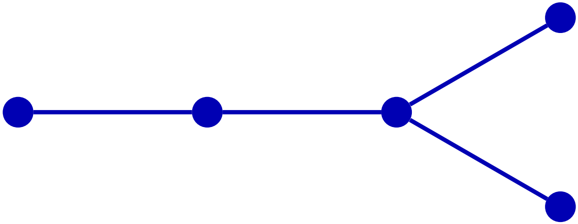
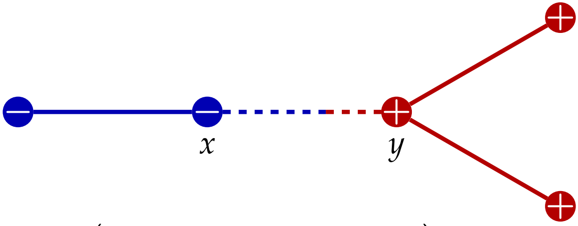


$$L(T) = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 3 & -1 & -1 \\ 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & -1 & 0 & 1 \end{pmatrix}$$

Example – Fiedler Vector



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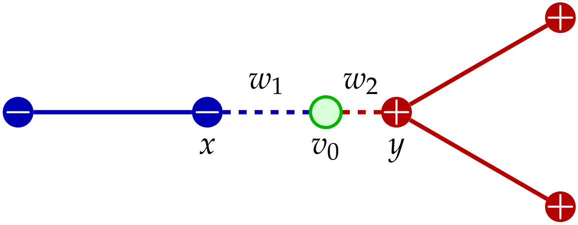
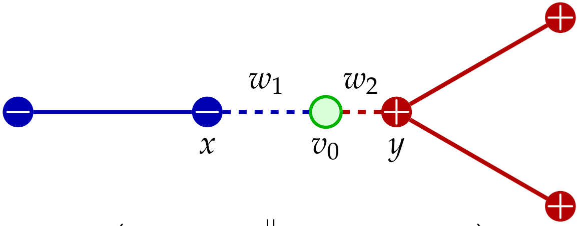
Example – Split



$$w_1 = |f(y) - f(x)| / |f(x)|$$
$$w_2 = |f(y) - f(x)| / |f(y)|$$

Example – Split



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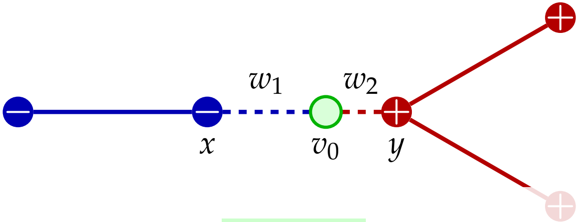
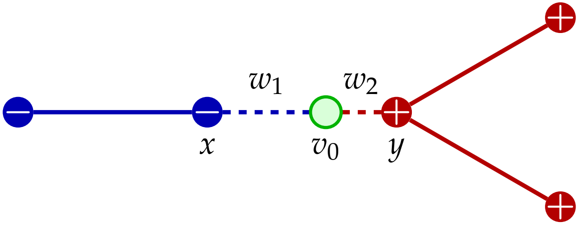


$$L(T') = \begin{pmatrix} 1 & -1 & 0 & 0 & 0 & 0 \\ -1 & 1+w_1 & -w_1 & 0 & 0 & 0 \\ 0 & -w_1 & w_1+w_2 & -w_2 & 0 & 0 \\ 0 & 0 & -w_2 & 2+w_2 & -1 & -1 \\ 0 & 0 & 0 & -1 & 1 & 0 \\ 0 & 0 & 0 & -1 & 0 & 1 \end{pmatrix}$$

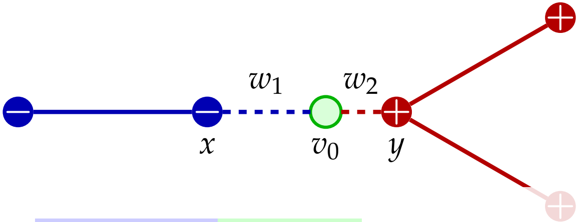
Example – Split



The algebraic connectivities of T and T' coincide.

$$\lambda_2(T) = \lambda_2(T')$$

Example – Nodal Domains



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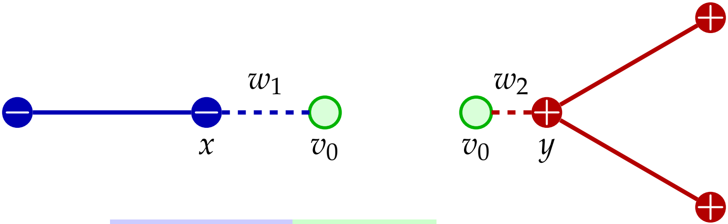

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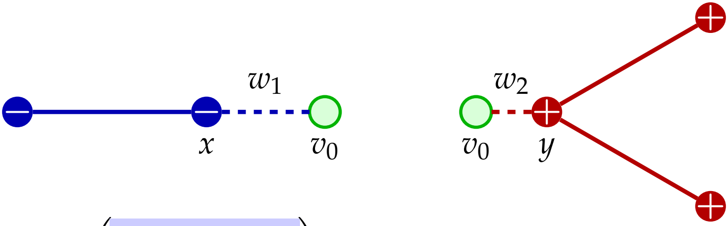
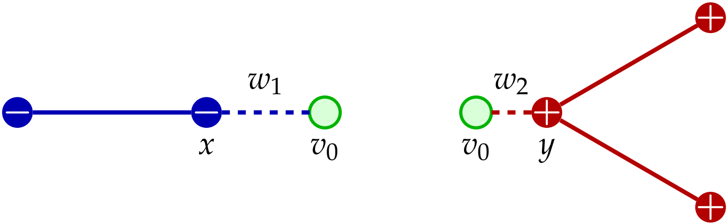
Example – Dirichlet Matrix



$$L^\circ(T_n) = \begin{pmatrix} 1 & -1 \\ -1 & 1+w_1 \end{pmatrix}$$

$$L^\circ(T_p) = \begin{pmatrix} 2+w_2 & -1 & -1 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{pmatrix}$$

Example – Dirichlet Matrix



The algebraic connectivity of T and
the first Dirichlet eigenvalues of T_n and T_p
coincide.

$$\lambda_2(T) = \nu(T_n) = \nu(T_p)$$

Local Eigenvalues

Let $G_1, \dots, G_k$ be graphs with boundaries.

Construct a new tree G without boundary by identifying boundary vertices of these trees and turning the boundary vertices into interior ones. Then

$$\lambda_k(G) \leq \max(\nu(G_1), \dots, \nu(G_k))$$

The inequality is strict if $\nu(G_i) \neq \nu(G_j)$ for some i, j.

Proof:

$$\frac{x_1 + \cdots + x_k}{y_1 + \cdots + y_k} \leq \max_{i=1,\dots,k} \frac{x_i}{y_i}$$

where equality holds if and only if $\frac{x_1}{y_2} = \cdots = \frac{x_k}{y_k}$.

Local Eigenvalues

Proof (cont.):

- Extend Perron vector g_i for each graph G_i on G by $g_i(v) = 0$ by $v \notin G_i$.
- Construct $f = \sum_{i=1}^{k} a_i g_i \neq 0$, such that $f \perp f_j$ for $j = 1, \ldots, k-1$.
- Courant-Fischer Theorem

$$\begin{aligned} \lambda_k(T) &\leq \frac{\sum_{i=1}^{k} \sum_{uv \in E_i} w_{uv}\, a_i^2 (g_i(u) - g_i(v))^2}{\sum_{i=1}^{k} \sum_{v \in V_i} a_i^2 g_i(v)^2} \\ &\leq \frac{\sum_{uv \in E_1} w_{uv}\, (g_1(u) - g_1(v))^2}{\sum_{v \in V_1} g_1(v)^2} = \nu(G_1) \end{aligned}$$

where we assume $\nu(G_1) \geq \nu(G_i)$.

Local Structures

Assume:
Eigenfunction f_k corresponding to the **simple** eigenvalue λ_k has (at least) k geometric nodal domains, $G_1, \ldots, G_k$.

For each G_i let $g_i = f_k\big|_{\mathcal{G}_i}$ and

- rearrange edges, and
- compare Rayleigh quotients of g_i on both G_i and G_i'.

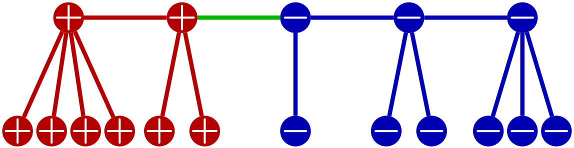
As we now have **first** Dirichlet eigenvalues, we are looking at unconstraint minima of the Rayleigh quotient.

Thus each geometric nodal domain of an extremal graph G is extremal.

Example

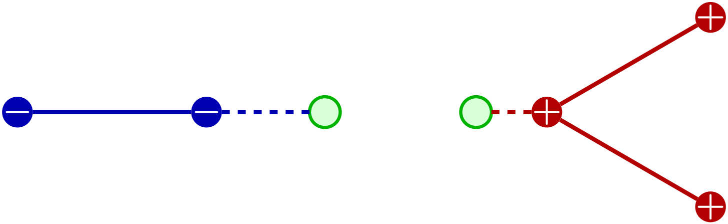
Algebraic Connectivity of Trees:

Let $\mathcal{T}_\pi$ the class of all trees with prescribed degree sequence π. If a tree T has minimal algebraic connectivity in $\mathcal{T}_\pi$, then T is a caterpillar. The degrees on the trunk vertices are decreasing from the end to the center. [Bıyıkoğlu and L, 2009]



Outline of Proof

- The Fiedler vector f has exactly **two** nodal domains T_n and T_p [Fiedler, 1975].
- On every path starting at point where f vanishes is either strictly **increasing**, decreasing or constant zero.



$$\lambda_2(T') \leq \max(\nu(T'_n), \nu(T'_p))$$

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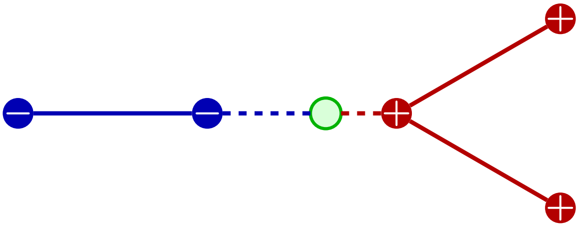

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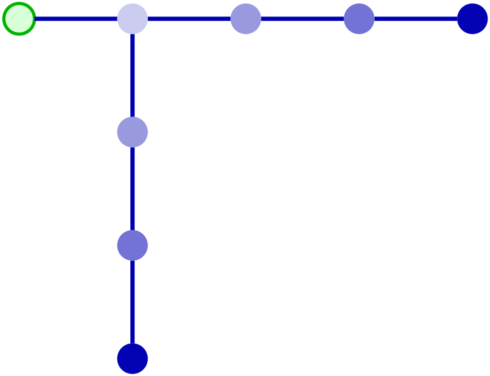
- Each nodal domain of an extremal tree must be a caterpillar. Otherwise shift branches (but leave pendant vertex) and thus decrease the Rayleigh quotient.



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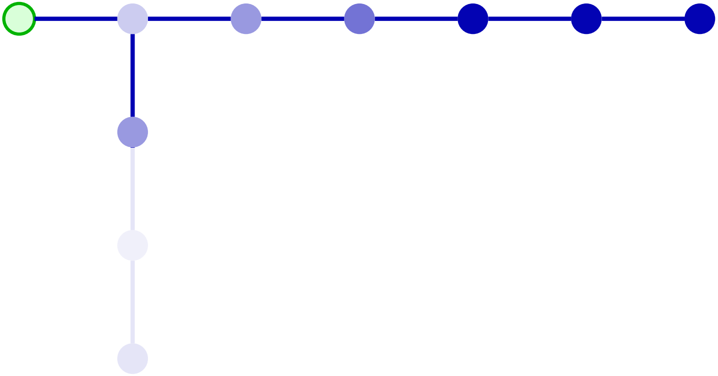
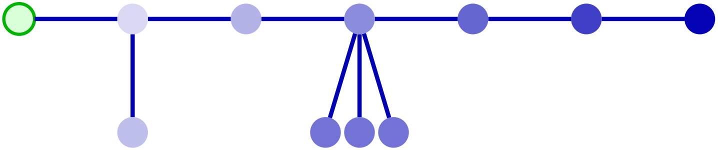


Outline of Proof

- Each nodal domain of an extremal tree must be a caterpillar. Otherwise shift branches (but leave pendant vertex) and thus decrease the Rayleigh quotient.
- The vertex degrees must be monotone. Otherwise shift pendant vertex away from boundary vertex and thus decrease the Rayleigh quotient.



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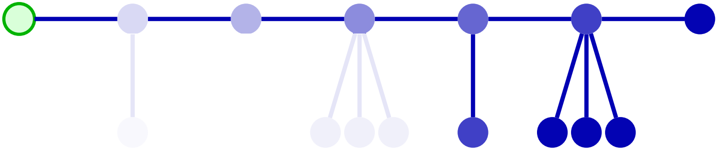

Remark

By this approach we cannot make global characterizations.

In our example:
It is not known how the degree sequence has to be split for the two nodal domains of the Fiedler vector.

Thank You

References I

Xiao-Dong Zhang. The Laplacian spectral radii of trees with degree sequences. *Discrete Mathematics*, 308(15):3143–3150, 2008. doi: doi:10.1016/j.disc.2007.06.017.

Joel Friedman. Some geometric aspects of graphs and their eigenfunctions. *Duke Math. J.*, 69(3):487–525, 1993.

Türker Bıyıkoğlu, Josef Leydold, and Peter F. Stadler. *Laplacian Eigenvectors of Graphs. Perron-Frobenius and Faber-Krahn Type Theorems*, volume 1915 of *Lecture Notes in Mathematics*. Springer, 2007.

Steve Kirkland, Michael Neumann, and Bryan L. Shader. Characteristic vertices of weighted trees via Perron values. *Linear Multilinear Algebra*, 40 (4):311–325, 1996.

T. Bıyıkoğlu and J. L. Algebraic connectivity and degree sequences of trees. *Linear Algebra and its Applications*, 430(2–3):811–817, 2009. doi: 10.1016/j.laa.2008.09.030.

References II

Miroslav Fiedler. A property of eigenvectors of nonnegative symmetric matrices and its application to graph theory. *Czechoslovak Math. J.*, 25: 619–633, 1975.