Numerical Computation of Equilateral Quantum Graph Spectra

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Introduction

A Quantum Graph [BK] consists of:

Metric Graph: $\mathcal{G} = (\mathcal{V}, \mathcal{E})$ with vertex set $\mathcal{V}$, edge set $\mathcal{E}$ and each edge e has same length ℓ

Hamiltonian: Negative second-order derivative on each edge: $\mathcal{H}: u(x) \mapsto -\frac{d^2u}{dx^2}$

Neumann-Kirchhoff Conditions: $u(x)$ is continuous on Γ and $\sum_{e \in \mathcal{E}_v} \frac{d}{dx} u|_e(v) = 0$ for all $v \in \mathcal{V}$

Vertex Eigenvalues and Eigenfunctions

Relation to combinatorial graph spectrum:

For $\sin(\sqrt{\lambda}\ell) \neq 0 \rightsquigarrow \lambda$ is eigenvalue of Γ corresponding to eigenfunction ϕ defined by

$$\phi_e = \frac{1}{\sin(\sqrt{\lambda}\ell)} \Big(\Phi(v_i) \sin(\sqrt{\lambda}(\ell - x)) + \Phi(v_j) \sin(\sqrt{\lambda} x) \Big) \text{ for all edges } e = (v_i, v_j)$$

$$\Longleftrightarrow$$

$\mu = (1 - \cos(\sqrt{\lambda}\ell))$ is eigenvalue of $\Delta_{\mathcal{G}}$ corresponding to eigenvector $\Phi = (\Phi(v_1), \ldots, \Phi(v_n))^T$

Rule to calculate Eigenvalues and -vectors:

Any vertex eigenvalue λ and associated vertex eigenfunction ϕ can be determined as

$$\lambda_{\mu,k} = \begin{cases} \left(\frac{1}{\ell}(\arccos(1-\mu) + k\pi)\right)^2 & \text{for } k \text{ even} \\ \left(\frac{1}{\ell}(\arccos(1-\mu) - (k+1)\pi)\right)^2 & \text{for } k \text{ odd} \end{cases}$$

and

$$(\phi_{\mu,k})_e(x) = \frac{1}{\sin\left(\sqrt{\lambda_{\mu,k}}\ell\right)} \left(\Phi(v_i) \sin\left(\sqrt{\lambda_{\mu,k}}(\ell - x)\right) + \Phi(v_j) \sin\left(\sqrt{\lambda_{\mu,k}} x\right) \right),$$

where (μ, Φ) is an eigenpair of $\Delta_{\mathcal{G}}$ with $\mu \notin \{0, 2\}$ and $k \in \mathbb{N}_0$

Example:

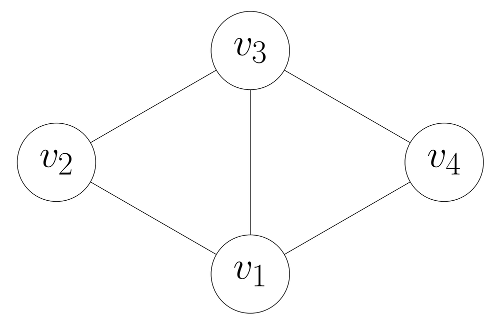

Figure 1: 4-cycle graph with one inner edge $\Gamma_{4,5}$ and equilateral edge length $\ell = 1$

- $\boldsymbol{D}$ = Degree-Matrix and $\mathcal{L}$ = Laplacian-Matrix
- Harmonic Laplacian-Matrix $\Delta_G \sim$ Symmetric Laplacian-Matrix $\mathcal{L}_{sym}$
  $\Rightarrow$ Spectrum of Δ_G and $\mathcal{L}_{sym}$ are identical

Harmonic Laplacian-Matrix:

$$\Delta_G = \boldsymbol{D}^{-1}\mathcal{L} = \begin{pmatrix} 1 & -\frac{1}{3} & -\frac{1}{3} & -\frac{1}{3} \\ -\frac{1}{2} & 1 & -\frac{1}{2} & 0 \\ -\frac{1}{3} & -\frac{1}{3} & 1 & -\frac{1}{3} \\ -\frac{1}{2} & 0 & -\frac{1}{2} & 1 \end{pmatrix}$$

Symmetric Laplacian-Matrix:

$$\mathcal{L}_{sym} = \boldsymbol{D}^{-1/2}\mathcal{L}\boldsymbol{D}^{-1/2} = \begin{pmatrix} 1 & -\frac{\sqrt{6}}{6} & -\frac{1}{3} & -\frac{\sqrt{6}}{6} \\ -\frac{\sqrt{6}}{6} & 1 & -\frac{\sqrt{6}}{6} & 0 \\ -\frac{1}{3} & -\frac{\sqrt{6}}{6} & 1 & -\frac{\sqrt{6}}{6} \\ -\frac{\sqrt{6}}{6} & 0 & -\frac{\sqrt{6}}{6} & 1 \end{pmatrix}$$

- Eigenvalues of $\mathcal{L}_{sym}$ are

$$\mu_1 = 0, \quad \mu_2 = 1, \quad \mu_3 = \frac{4}{3}, \quad \mu_4 = \frac{5}{3}$$

- Eigenvectors of $\mathcal{L}_{sym}$ are

$$\Phi_1 = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}, \quad \Phi_2 = \begin{pmatrix} 0 \\ -1 \\ 0 \\ 1 \end{pmatrix}, \quad \Phi_3 = \begin{pmatrix} -1 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad \Phi_4 = \begin{pmatrix} -\frac{2}{3} \\ 1 \\ -\frac{2}{3} \\ 1 \end{pmatrix}$$

- $\mu_1 = 0$ does not correspond to vertex eigenvalue $\rightsquigarrow \sin(0) = 0$

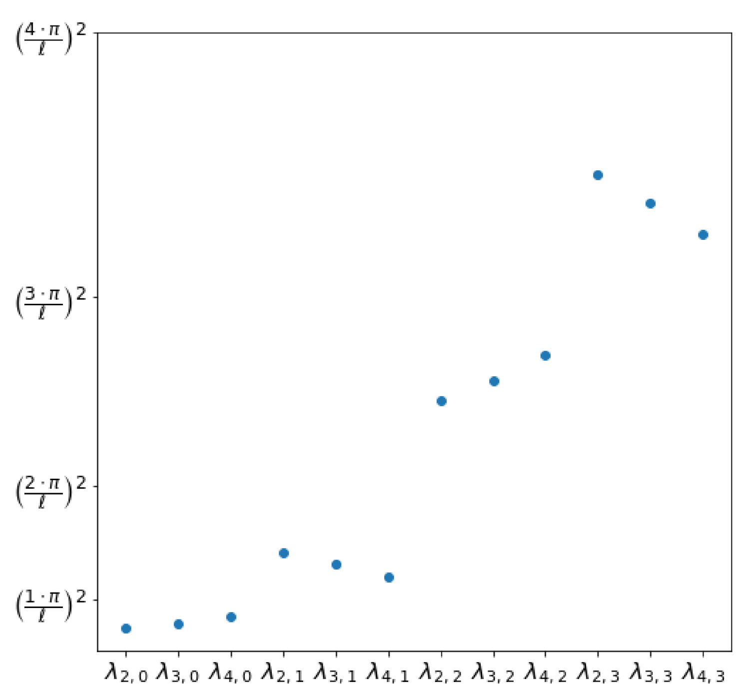

Figure 2: Vertex Eigenvalues of Γ for $k = 0, \ldots, 3$

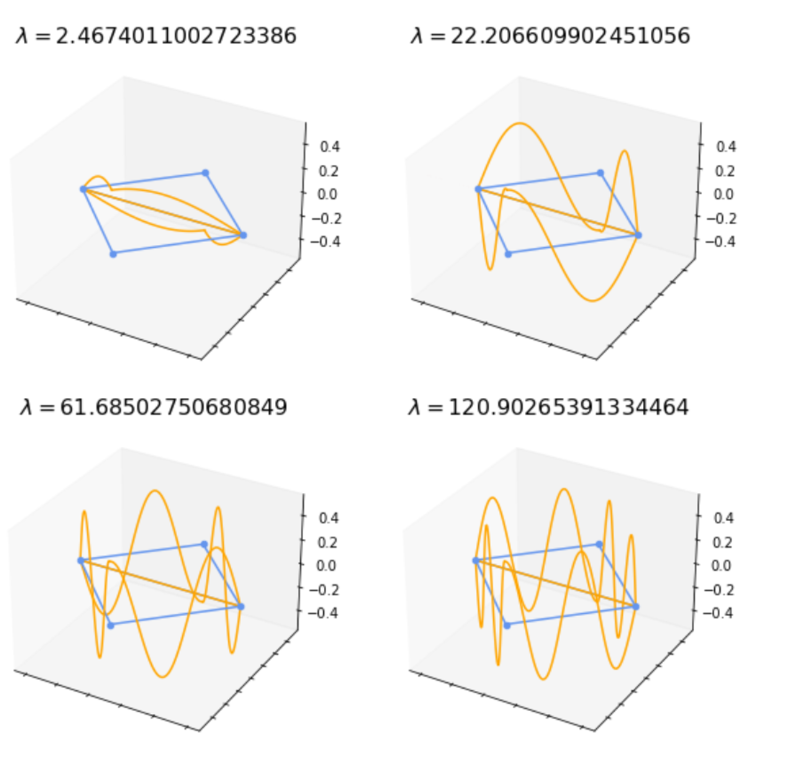

Figure 3: Vertex Eigenfunctions of Γ for μ_2 for $k = 0, \ldots, 3$ [W]

Non-Vertex Eigenvalues

- Eigenvalues of the form $\left(\frac{k\pi}{\ell}\right)^2$, $k \in \mathbb{Z}$ are called non-vertex eigenvalues
- If $\lambda = \left(\frac{k\pi}{\ell}\right)^2$, $k \in \mathbb{Z}$ applies, then $\sin(\sqrt{\lambda}\ell) = 0 \rightsquigarrow$ therefore, we cannot use our relation
- Let $\Gamma = (\mathcal{V}, \mathcal{E}, \ell)$ be metric graph with edge lengths ℓ
- Consider extended graph $\tilde{\Gamma}_k := (\tilde{\mathcal{V}}, \tilde{\mathcal{E}}, \ell/(k+1))$ that arises from insertion of k artificial vertices on each edge $e \in \mathcal{E}$
- Every non-vertex eigenvalue $\lambda = \left(\frac{k\pi}{\ell}\right)^2$ of metric graph Γ with length ℓ is vertex eigenvalue of extended graph $\tilde{\Gamma}_k$ with k artificial vertices on each edge [AW]

Multiplicity of non-vertex eigenvalues:

The multiplicity of $\lambda = \left(\frac{k\pi}{\ell}\right)^2$ as an eigenvalue of Γ is given by

$$\begin{cases} 1 & \text{if } k = 0 \\ m - n + 2 & \text{if } k \text{ even} \\ m - n & \text{if } k \text{ odd and } \Gamma \text{ not bipartite} \\ m - n + 2 & \text{if } k \text{ odd and } \Gamma \text{ bipartite} \end{cases}$$

where $n = |\mathcal{V}|$ and $m = |\mathcal{E}|$ of Γ.

Non-vertex eigenvalues:

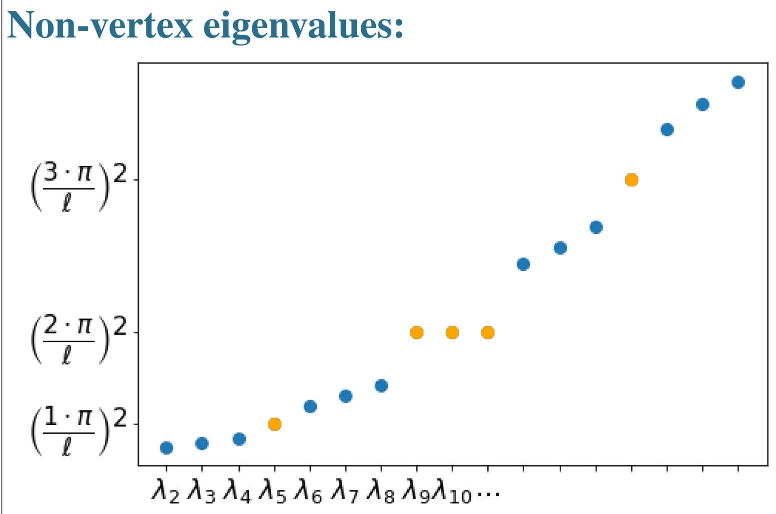

Figure 4: Spectrum of $\tilde{\Gamma}_3$: orange dots represent non-vertex eigenvalues, blue dots represent vertex eigenvalues

Non-vertex eigenvectors:

Since $\lambda = \left(\frac{k\pi}{\ell}\right)^2$ is vertex eigenvalue of $\tilde{\Gamma} \rightsquigarrow$ eigenfunctions can be determined with eigenvectors of $\tilde{\Gamma}$:

$$\phi_e(x) = \tilde{\Phi}(v_i) \cos\left(\frac{k\pi}{\ell}x\right) + \frac{1}{\sin\left(\frac{k}{k+1}\pi\right)} \left(\tilde{\Phi}(v_{e,1}) - \tilde{\Phi}(v_i) \cos\left(\frac{k}{k+1}\pi\right) \right) \sin\left(\frac{k\pi}{\ell}x\right)$$

where $v_{e,1}$ is first artificial vertex on edge $e \rightsquigarrow$ find all eigenvectors corresponding to $\lambda = \left(\frac{k\pi}{\ell}\right)^2$

Through our relation we get:

$$\tilde{\mathcal{L}}_{sym_k}\tilde{\Phi} = \left(1 - \cos\sqrt{\lambda}\tilde{\ell}\right)\tilde{\Phi} \Longleftrightarrow \left(\tilde{\mathcal{L}}_{sym_k} - \left(1 - \cos\frac{k\pi}{k+1}\tilde{\ell}\right)\mathcal{I}\right)\tilde{\Phi} = 0$$

$\rightsquigarrow$ need kernel of the matrix $\tilde{\mathcal{L}}_{sym_k} - \left(1 - \cos\frac{k\pi}{k+1}\tilde{\ell}\right)\mathcal{I}$.

- Compute kernel by singular value decomposition [DR]
- Matrix $\tilde{\mathcal{L}}_{sym_k}$ and $\tilde{\Phi}$ can be written as: $\tilde{\mathcal{L}}_{sym_k} = \begin{bmatrix} \mathcal{I}_{n \times n} & \tilde{\mathcal{L}}_{\mathcal{V}\mathcal{E}} \\ \tilde{\mathcal{L}}_{\mathcal{E}\mathcal{V}} & \tilde{\mathcal{L}}_{\mathcal{E}\mathcal{E}} \end{bmatrix}$ and $\tilde{\Phi} = \begin{bmatrix} \tilde{\Phi}_{\mathcal{V}} \\ \tilde{\Phi}_{\mathcal{E}} \end{bmatrix}$

For $\tilde{\Phi}_{\mathcal{V}}$ we distinguish three cases:

- If k is odd, Γ not bipartite $\rightsquigarrow \tilde{\Phi}_{\mathcal{V}} \equiv 0$
- If k is even $\rightsquigarrow \tilde{\Phi}_{\mathcal{V}} = c \cdot \boldsymbol{D}^{1/2}\mathbf{1}$, for $c \in \mathbb{R}$
- If k is odd, Γ is bipartite $\rightsquigarrow \tilde{\Phi}_{\mathcal{V}} = c \cdot \boldsymbol{D}^{1/2}\Phi_n$, for $c \in \mathbb{R}$ and Φ_n eigenvector corresponding to eigenvalue 2

By taking advantage of properties from $\tilde{\Phi}_{\mathcal{V}}$, computing time can be decreased by roughly 30%

Singular value decomposition of	Solution time in sec.
initial system	142.089
new system	103.747

Table 1: Time to compute singular value decomposition in Julia for $|\tilde{\mathcal{V}}| = 5899$

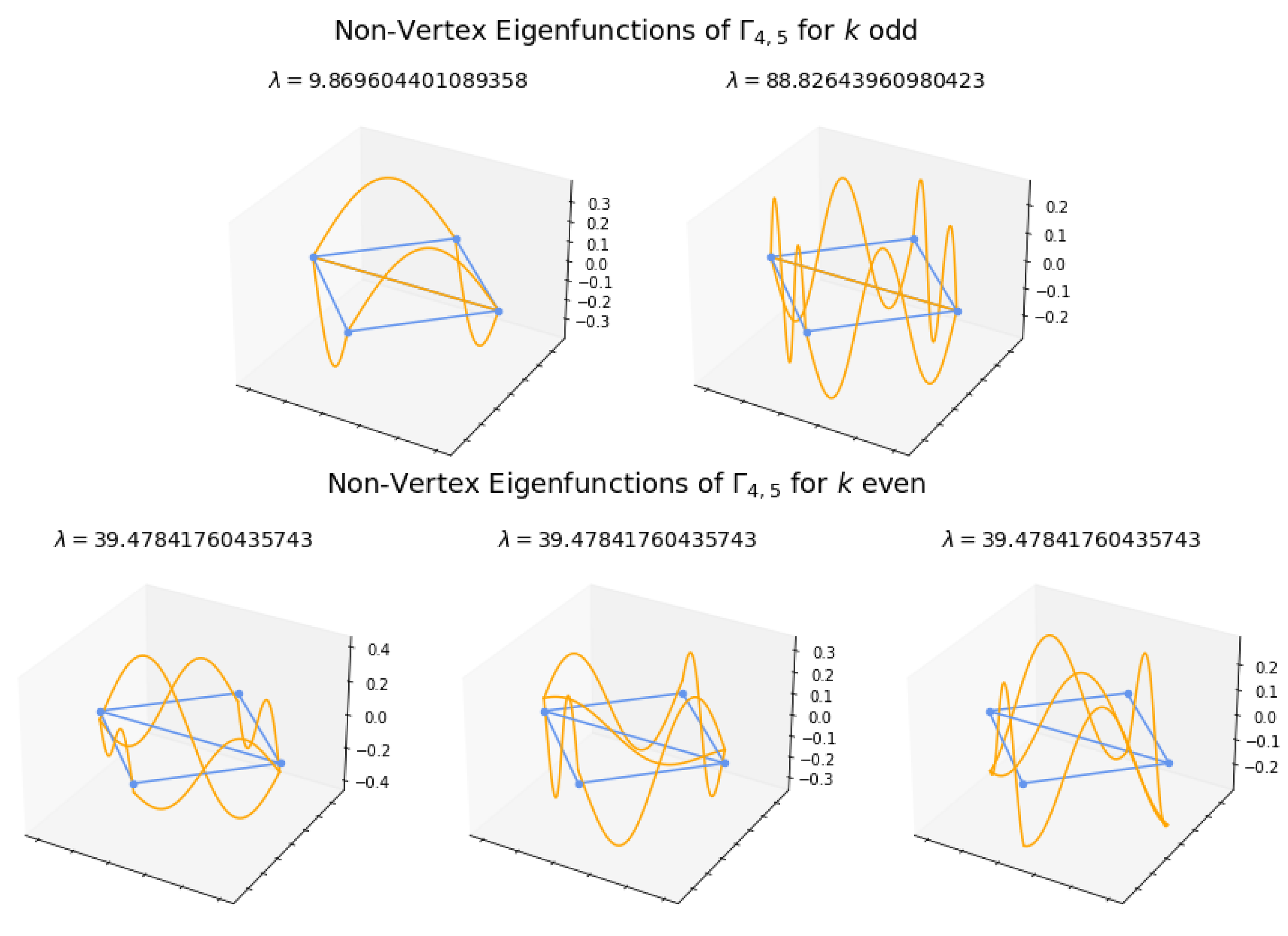

Figure 5: Non-Vertex Eigenfunctions of $\Gamma_{4,5}$ for k even and odd [W]

References

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