MAT 280: Harmonic Analysis on Graphs & Networks
Lecture 8: Graph Laplacian Eigenfunctions III: Analysis of Localization/Phase Transition Phenomena

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Outline

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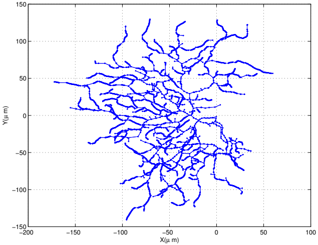
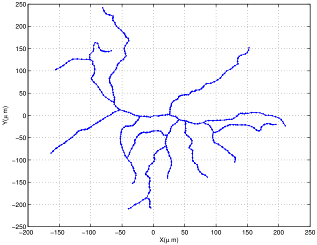
A Peculiar Phase Transition Phenomenon

Recall the interesting *phase transition* phenomenon of the graph Laplacian eigenvalues and eigenfunctions on dendritic trees mentioned in Lecture 5.



(a) RGC #60



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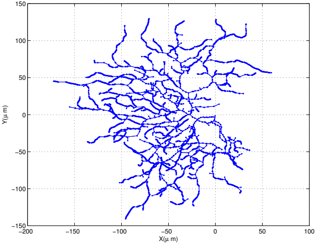

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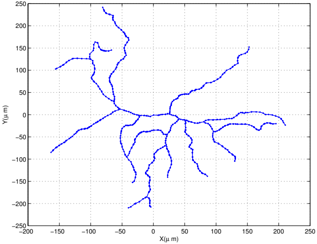

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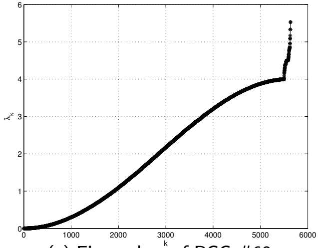
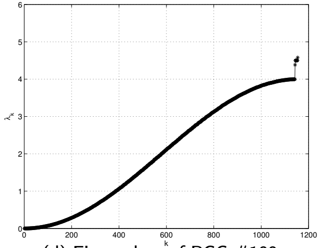


(c) Eigenvalues of RGC #60



(d) Eigenvalues of RGC #100

A Peculiar Phase Transition Phenomenon ...

We have observed that this value 4 is critical since:

- the eigenfunctions corresponding to the eigenvalues below 4 are *semi-global* oscillations (like Fourier cosines/sines) over the entire dendrites or one of the dendrite arbors;
- those corresponding to the eigenvalues above 4 are much more *localized* (like wavelets) around junctions/bifurcation vertices.

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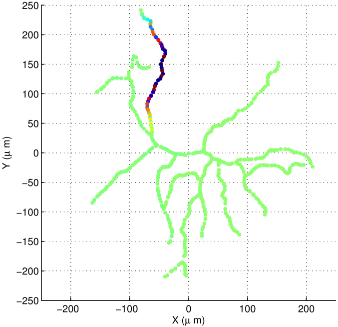

(a) RGC #100; $\lambda_{1141} = 3.9994$

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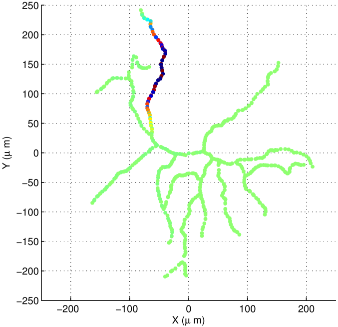

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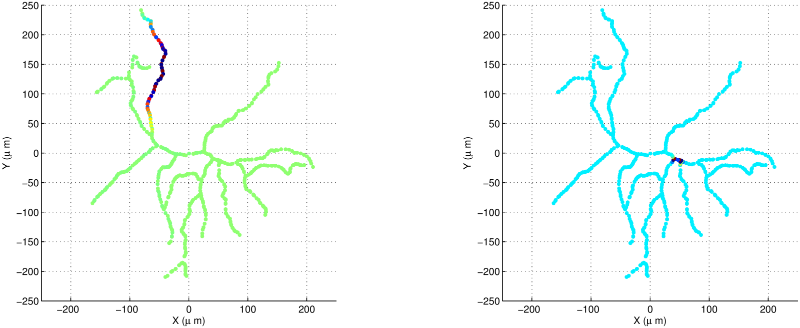

(a) RGC #100; $\lambda_{1141} = 3.9994$

(b) RGC #100; $\lambda_{1142} = 4.3829$

Natural Questions

Q1 Why does such a phase transition phenomenon occur?

Q2 What is the significance of the eigenvalue 4?

Q3 Is there any tree that possesses an eigenvalue exactly equal to 4?

Q4 What about more general graphs that possess eigenvalues exactly equal to 4?

Q5 How about trees with edge weights?

- Analyzing data measured on not only dendritic trees but also general graphs
- Building/designing *wavelet-like* analysis/synthesis tools on graphs

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A Starlike Tree

It is a good idea to start our analysis on trees much simpler than the real dendritic trees. A *starlike tree* is such a model where there is only one vertex whose degree is larger than 2.

- Let $S(n_1, n_2, \ldots, n_k)$ be a starlike tree that has $k(\geq 3)$ paths (i.e., branches) emanating from the center vertex v_1.
- Let the ith branch have n_i vertices excluding v_1.
- Let $n_1 \geq n_2 \geq \cdots \geq n_k$.
- The total number of vertices: $n = 1 + \sum_{i=1}^{k} n_i$.

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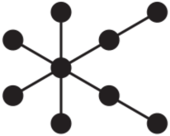

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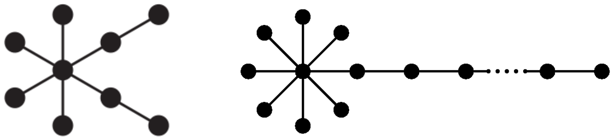

(a) $S(2,2,1,1,1,1)$ **(b)** $S(n_1,1,1,1,1,1,1,1)$ a.k.a. comet

Known Results on Starlike Trees

- We proved (in 2010) the largest eigenvalue for a comet is always larger than 4.
- K. Ch. Das (2007) proved the following results.
  - $\lambda_{\max} = \lambda_{n-1} < k + 1 + \dfrac{1}{k-1}$
  - $2 + 2\cos\left(\dfrac{2\pi}{2n_k + 1}\right) \le \lambda_{n-2} \le 2 + 2\cos\left(\dfrac{2\pi}{2n_1 + 1}\right)$
- On the other hand, Grone and Merris (1994) proved the following lower bound for a general graph G with at least one edge:

$$\lambda_{\max} \ge \max_{1\le j\le n} d(v_j) + 1.$$

Our Results on Starlike Trees

Corollary (S-Woei 2010)

A starlike tree has exactly one graph Laplacian eigenvalue greater than or equal to 4. *The equality holds if and only if the starlike tree is* $K_{1,3} = S(1,1,1)$, *which is also known as a claw.*

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Theorem (S-Woei 2011)

Let $\boldsymbol{\phi}_{n-1} = \left(\phi_{1,n-1}, \cdots, \phi_{n,n-1}\right)^{\mathsf{T}}$, *where* $\phi_{j,n-1}$ *is the value of the eigenfunction corresponding to the largest eigenvalue* λ_{n-1} *at the vertex* v_j, $j = 1, \ldots, n$. *Then, the absolute value of this eigenfunction at the central vertex* v_1 *cannot be exceeded by those at the other vertices, i.e.,*

$$|\phi_{1,n-1}| > |\phi_{j,n-1}|, \quad j = 2, \ldots, n.$$

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$$|\phi_{1,n-1}| > |\phi_{j,n-1}|, \quad j = 2, \ldots, n.$$

The proof is based on *Geršgorin's Theorem*.

Geršgorin's Theorem (1931)

Consider any $A = (a_{ij}) \in \mathbb{C}^{n \times n}$, and define

$$\begin{aligned} N &:= \{1, \ldots, n\}, \\ r_i(A) &:= \sum_{j \in N \setminus \{i\}} |a_{ij}|, \\ \Gamma_i(A) &:= \{z \in \mathbb{C} : |z - a_{ii}| \le r_i(A)\}, \\ \Gamma(A) &:= \bigcup_{i \in N} \Gamma_i(A). \end{aligned}$$

Then for any $\lambda \in \sigma(A)$, there is a positive integer $k \in N$ such that

$$|\lambda - a_{kk}| \le r_k(A).$$

Consequently, $\lambda \in \Gamma_k(A) \subseteq \Gamma(A)$. Hence,

$$\sigma(A) \subseteq \Gamma(A).$$

Proof of Theorem of S-Woei 2011

To prove this theorem, we use the following lemma:

Lemma

Let $A \in \mathbb{C}^{n\times n}$, $\lambda_k(A)$ be any eigenvalue of A, and $\boldsymbol{\phi}_k = (\phi_{1,k}, \ldots, \phi_{n,k})^{\mathsf{T}}$ be the corresponding eigenvector. Let k^* denote the index of the largest eigenvector component in $\boldsymbol{\phi}_k$, i.e., $\left|\phi_{k^*,k}\right| = \max_{j\in N}\left|\phi_{j,k}\right|$. Then, we must have $\lambda_k(A) \in \Gamma_{k^*}(A)$. In other words, for the index of the largest eigenvector component, the corresponding Geršgorin disk must contain the eigenvalue.

Proof. We follow the usual proof of Geršgorin's theorem. The k^*th row of $A\boldsymbol{\phi}_k = \lambda_k \boldsymbol{\phi}_k$ yields

$$|\lambda_k - a_{k^*k^*}| \le \sum_{j\in N\setminus\{k^*\}} \left|a_{k^*j}\right| \frac{\left|\phi_{j,k}\right|}{\left|\phi_{k^*,k}\right|} \le \sum_{j\in N\setminus\{k^*\}} \left|a_{k^*j}\right|.$$

This implies $\lambda_k \in \Gamma_{k^*}(A)$, which proves the lemma. □

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Let us now prove the target theorem. First of all, by Corollary (S-Woei 2011), we have $\lambda_{n-1} \geq 4$. However, $\lambda_{n-1} = 4$ happens only for $K_{1,3}$. In that case, it is easy to see that this theorem holds by directly examining the eigenvector $\boldsymbol{\phi}_{n-1} = \boldsymbol{\phi}_3 \propto (3,-1,-1,-1)^\mathsf{T}$. Hence, let us examine the case $\lambda_{n-1} > 4$. In this case, the lemma indicates $4 < \lambda_{n-1} \in \Gamma_{(n-1)^*}(L)$ where $(n-1)^* \in N$ is the index of the largest component in $\boldsymbol{\phi}_{n-1}$. Now, note that the disk $\Gamma_i(L)$ for any vertex v_i that has degree 2 is $\{z \in \mathbb{C} : |z-2| \leq 2\}$ (and $\{z \in \mathbb{C} : |z-1| \leq 1\}$ for a degree 1 vertex). This means that the Geršgorin disk $\Gamma_{(n-1)^*}$ containing the eigenvalue $\lambda_{n-1} > 4$ cannot be in the union of the Geršgorin disks corresponding to the vertices whose degrees are 2 or less. Hence the index of the largest eigenvector component in $\boldsymbol{\phi}_{n-1}$ must correspond to an index for which the vertex has degree 3 or larger. In our starlike-tree case, there is only one such vertex, v_1, i.e., $(n-1)^* = 1$. □

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Why Is the Eigenvalue 4 Critical on Starlike Trees? (Q2)

- The eigenvalue equation along each branch, say, the first branch containing n_1 vertices, leads to the following recursion formula:

$$\phi_{j+1} + (\lambda - 2)\phi_j + \phi_{j-1} = 0, \quad j = 2, \ldots, n_1$$

with the appropriate boundary condition.

- Consider its *characteristic equation* $r^2 + (\lambda - 2)r + 1 = 0$. Then, the general solution can be written as $\phi_j = Ar_1^{j-2} + Br_2^{j-2}$, $j = 2, \ldots, n_1 + 1$, where r_1, r_2 are the roots of the characteristic equation, and A, B are appropriate constants derived from the boundary condition.
- The discriminant of the characteristic equation is

$$\mathscr{D}(\lambda) := (\lambda - 2)^2 - 4 = \lambda(\lambda - 4).$$

- Hence if $0 \le \lambda < 4$, then $r_1, r_2 \in \mathbb{C}$, which give us the *oscillatory* solution, while if $\lambda > 4$, we can show $r_1 < -1 < r_2 < 0$, which lead to the *more concentrated* solution.

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Our Dataset

consists of 130 RGCs each of which in turn consists of

- A sequence of 3D sample points along dendrite arbors obtained by Neurolucida® (requires intensive human interaction)
- Connectivity and branching information by the same software
- Each soma (cell body) is represented as a sequence of points traced along its boundary (circular/ring shape)

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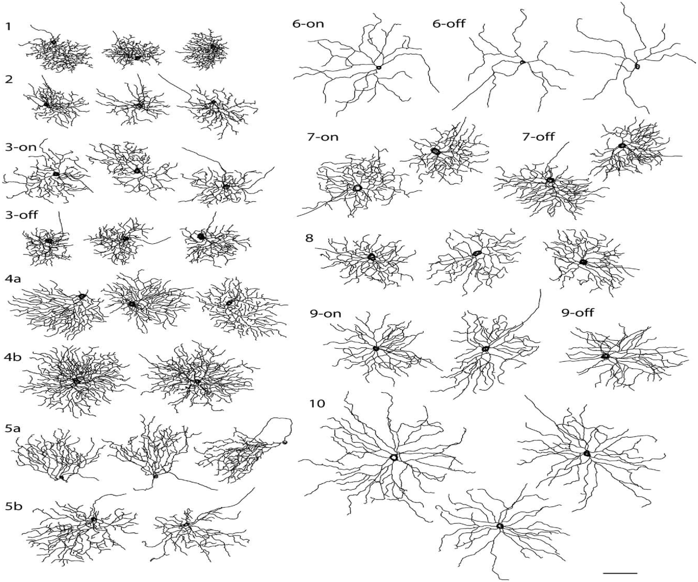
$\Longrightarrow$ Constructing a *graph* representing dendrite structures per RGC is very natural and simple! In fact, we constructed a *tree* (i.e., a connected graph without cycles/loops) by replacing the soma ring by a single vertex representing a center of the soma.

Recap: Clustering using Features Derived by Neurolucida®



Our Dataset $\Longrightarrow$ Trees . . .

- Let G be a *tree* representing dendrites of an RGC.
- Let $V = V(G) = \{v_1, \dots, v_n\}$ be a set of *vertices* representing sample points along dendrite arbors, i.e., $v_k \in \mathbb{R}^3$. n ranges between 565 and 24474 depending on the RGCs.
- Let $E = E(G) = \{e_1, \dots, e_{n-1}\}$ be a set of *edges* where $e_k = (v_i, v_j)$ represents a line segment connecting between adjacent vertices v_i, v_j for some $1 \le i, j \le n$.
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$$\max_{\text{130 cells}} \max_k d(v_k) = 8, \qquad \min_{\text{130 cells}} \max_k d(v_k) = 3.$$

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Our Observations via Numerical Experiments

- Unfortunately, actual dendritic trees are not starlike.
- However, our numerical computations and data analysis indicate that:

$$0 \le \frac{\#\{j \in [1,n] \,|\, d(v_j) \gneqq 2\} - m_G([4,\infty))}{n} \le 0.047$$

for each cell where $n = |V(G)|$.

- We can define the *starlikeliness* $S\ell(T)$ of a given tree $G = T$ as follows:

$$S\ell(T) := 1 - \frac{\#\{j \in [1,n] \,|\, d(v_j) \gneqq 2\} - m_T([4,\infty))}{n}.$$

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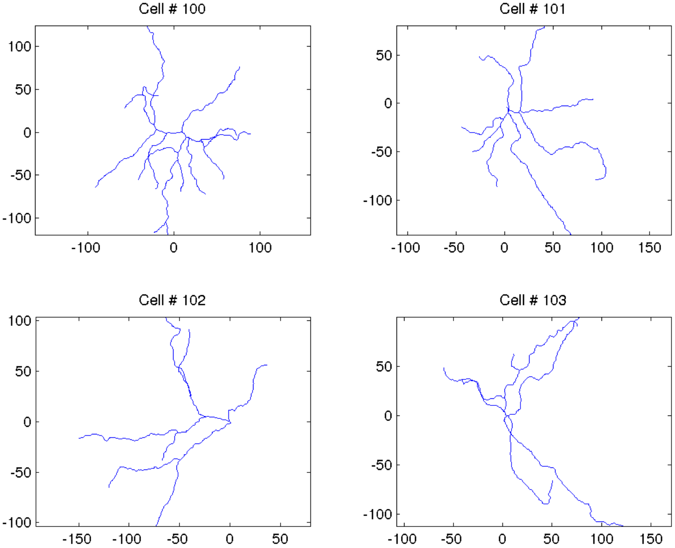
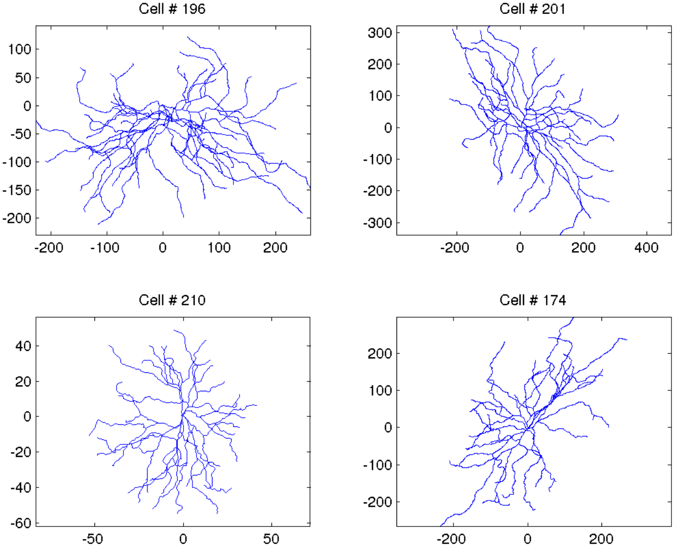
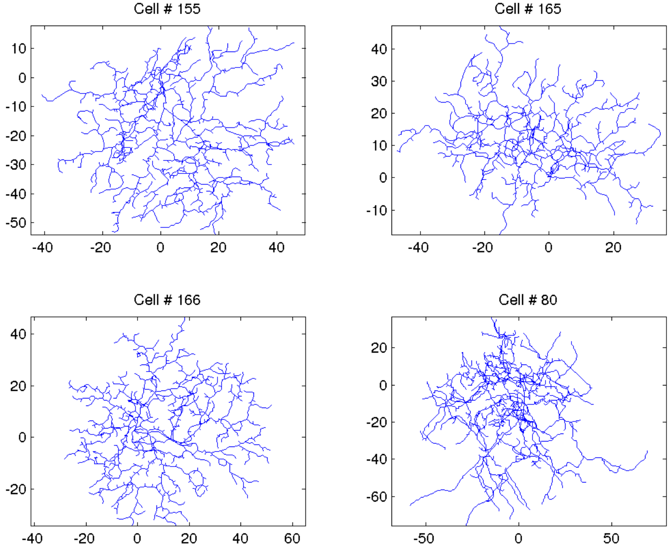
Dendrites with $S\ell(T) = 1$



More dendrites with $S\ell(T) = 1$



Dendrites with $S\ell(T) \lneq 1$



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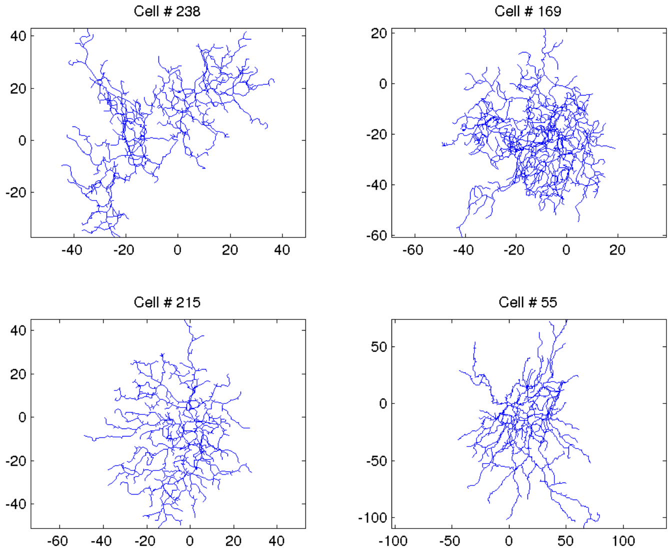
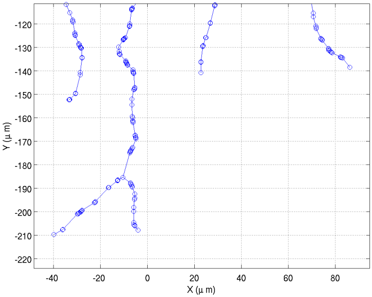
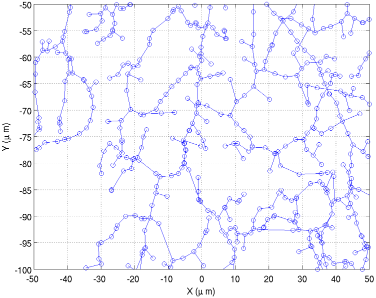


Zoom up



(a) RGC #100; $S\ell(T) = 1$



(b) RGC #155; $S\ell(T) = 0.953 \lneqq 1$

Observations $\Longrightarrow$ Theorems on General Graphs

Theorem (Nakatsukasa-S-Woei 2013)

For any graph G of finite volume, we have

$$0 \leq m_G([4,\infty)) \leq \#\{j \in [1,n] \mid d(v_j) \gneq 2\}$$

and each eigenfunction corresponding to $\lambda \geq 4$ has its largest component (in the absolute value) on the vertices whose degree are larger than 2.

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Theorem (Nakatsukasa-S-Woei 2013)

Suppose that a graph G has a branch consisting of a path of length k, say, $\{v_{i_1}, \ldots, v_{i_k}\}$ with v_{i_k} being the leaf of that branch. Then for any $\lambda > 4$, the corresponding eigenvector $\boldsymbol{\phi} = \left(\phi_1, \cdots, \phi_n\right)^{\mathsf{T}}$ satisfies

$$|\phi_{i_{j+1}}| \le \gamma |\phi_{i_j}| \quad \text{for } j = 1, 2, \ldots, k-1, \quad \gamma := 2/(\lambda - 2) < 1.$$

Hence $|\phi_{i_j}| \le \gamma^{j-1} |\phi_{i_1}|$ for $j = 1, \ldots, k$, that is, the eigenvector along the branch decays exponentially with the rate γ.

Outline

Answers to Q3

Theorem (Guo 2006)

Let T be a tree with n vertices. Then,

$$\lambda_j(T) \le \left\lceil \frac{n}{n-j} \right\rceil, \quad j = 0, \ldots, n-1,$$

and the equality holds iff a) $j \neq 0$; b) $n-j$ divides n; and c) T is spanned by $n-j$ vertex disjoint copies of $K_{1,\frac{j}{n-j}}$.

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Corollary (Nakatsukasa-S-Woei 2013)

A tree has an eigenvalue exactly equal to 4 iff it consists of vertex disjoint copies of $K_{1,3}$.

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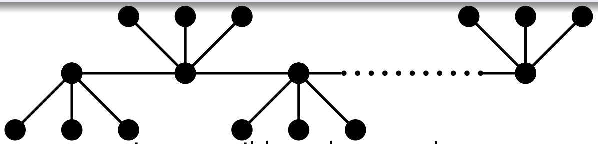
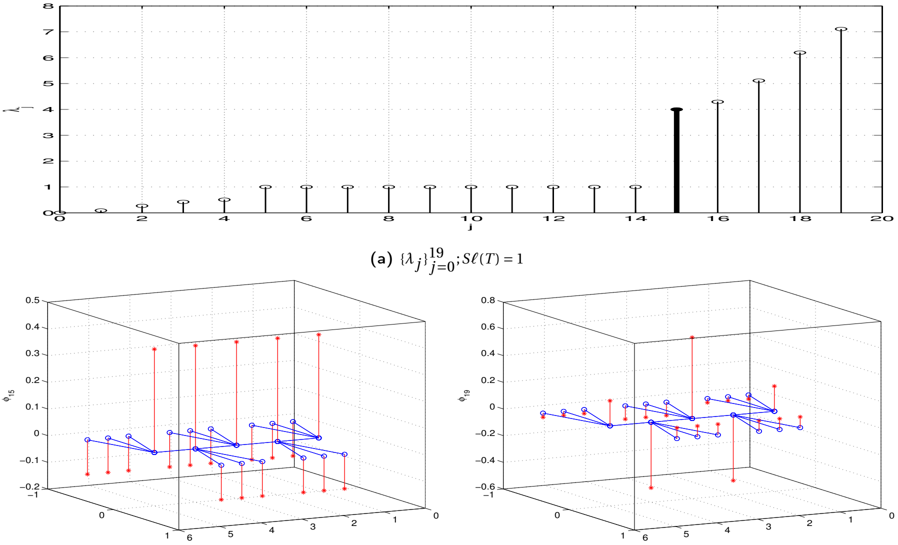


Many other connections possible as long as they are vertex disjoint.

Answers to Q3 . . .



(a) $\{\lambda_j\}_{j=0}^{19}; S\ell(T) = 1$

(b) ϕ_{15}

(c) ϕ_{19}

Outline

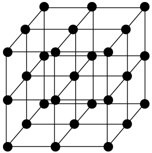
Q4: Can a graph have the eigenvalue $\lambda = 4$?

- The answer is clearly *Yes*: a regular finite lattice graph in $\mathbb{R}^d$, $d > 1$ has repeated eigenvalue 4.
- The eigenvalues and the corresponding eigenfunctions of a graph representing the regular finite lattice of size $n \times n \times \cdots \times n = n^d$ are

$$\lambda_{j_1,\dots,j_d} = 4 \sum_{i=1}^{d} \sin^2\left(\frac{j_i \pi}{2n}\right)$$

$$\phi_{j_1,\dots,j_d}(x_1,\dots,x_d) = \prod_{i=1}^{d} \cos\left(\frac{j_i \pi (x_i + \frac{1}{2})}{n}\right),$$

where $j_i, x_i \in \mathbb{Z}/n\mathbb{Z}$ for each i; see Burden and Hedstrom: "The distribution of the eigenvalues of the discrete Laplacian," *BIT*, vol.12, pp.475–488, 1972.



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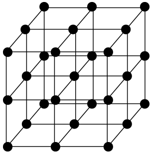

- Hence, determining $m_G(4)$ of this lattice graph is equivalent to finding the integer solution $(j_1, \ldots, j_d) \in (\mathbb{Z}/n\mathbb{Z})^d$ to the following equation:

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- For $d = 1$, $m_G(4) = 0$ as shown earlier.
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- For $d = 3$, $m_G(4)$ behaves in a much more complicated manner, which is deeply related to *Number Theory*.
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Q5: How about trees with edge weights?

- It turned out that even an extremely simple tree, i.e., a "path" can have localized eigenfunctions like wavelets if it has *non-uniform edge weights*.

A simple yet weighted path

Play/Pause

- Interesting to see that such non-uniform weights can generate both global oscillations like Fourier mode and localized wiggles like wavelets.
- This indicates that weighted graphs exhibit more unexpected yet interesting behaviors and their analysis will be more challenging compared to the unweighted (or combinatorial) graphs.

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Summary

- Obtained complete understanding of the eigenvalue/eigenfunction behavior for unweighted starlike trees
- Obtained a theorem on exponential amplitude decay of the eigenfunctions corresponding to the eigenvalues > 4
- Identified a class of trees having exact eigenvalue 4
- Lattice graphs can have exact eigenvalue 4 with multiplicity, but tough to analyze the relationship between $m_G(4)$ and the dimension d of the lattice $\Longrightarrow$ Analytic Number Theory!
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References, etc.

- Laplacian Eigenfunction Resource Page
https://www.math.ucdavis.edu/~saito/lapeig/ contains my course notes on the basics of Laplacian eigenfunctions
- Conferences & Workshops Resource Page
https://www.math.ucdavis.edu/~saito/confs/ contains information and talk slides of various minisymposia I organized including the minisymposium on "Harmonic Analysis on Graphs and Networks: Theory and Applications" at ICIAM 2011 (Vancouver, Canada).
- The following articles are available at
http://www.math.ucdavis.edu/~saito/publications/
* N. Saito and E. Woei: "Analysis of neuronal dendrite patterns using eigenvalues of graph Laplacians," *Japan SIAM Letters*, vol.1, pp.13-16, 2009.
* N. Saito and E. Woei: "On the phase transition phenomenon of graph Laplacian eigenfunctions on trees," *RIMS Kôkyûroku*, vol.1743, pp.77-90, 2011.
* Y. Nakatsukasa, N. Saito, and E. Woei: "Mysteries around graph Laplacian eigenvalue 4," *Linear Algebra and its Applications*, vol.438, pp.3231-3246, 2013.
* N. Saito and E. Woei: "Tree simplification and the 'plateaux' phenomenon of graph Laplacian eigenvalues," *Linear Algebra and its Applications*, vol.481, pp.263-279, 2015.

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