Mysteries Around Graph Laplacian Eigenvalue 4

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Outline

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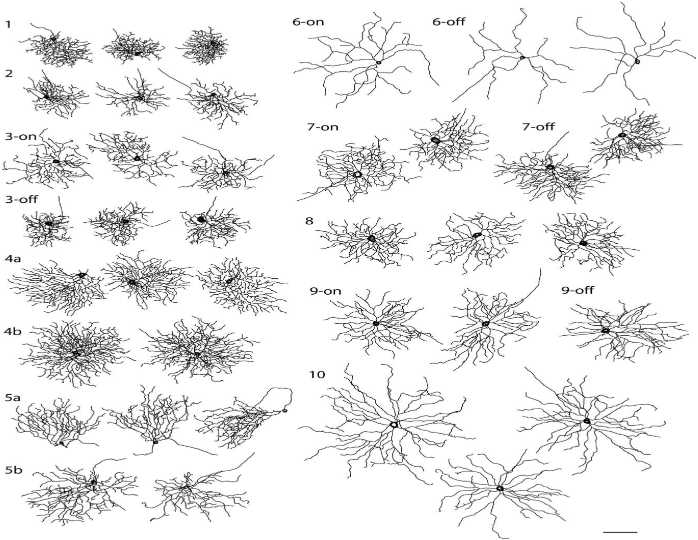
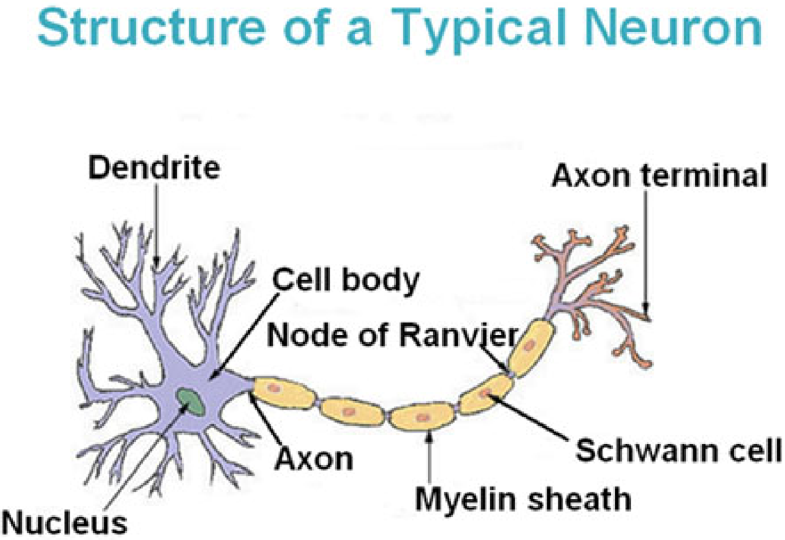
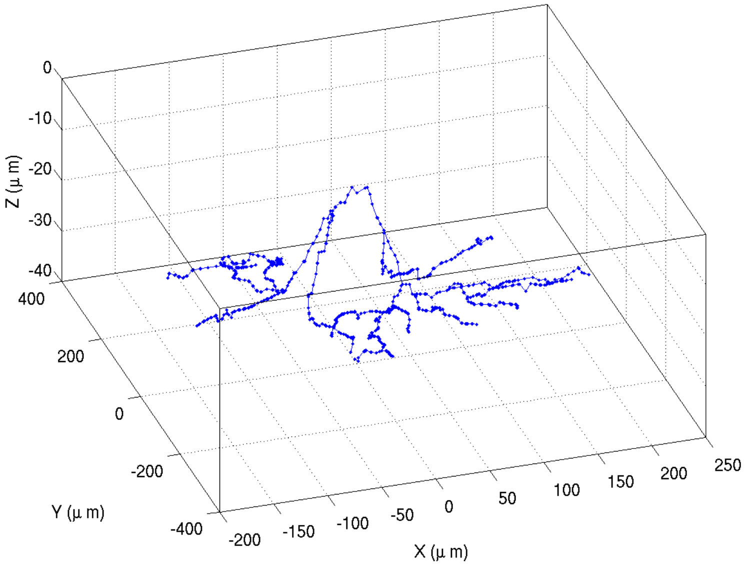
Morphological Analysis of Dendritic Trees of Mouse's Retinal Ganglion Cells



A Typical Neuron (from Wikipedia)



A Real Dendritic Tree Encoded as a Graph



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While we were analyzing the morphological features of the dendritic trees using the the eigenvalues and eigenfunctions of graph Laplacians defined on such trees, we observed an interesting phase-transition or thresholding phenomenon on their behavior.

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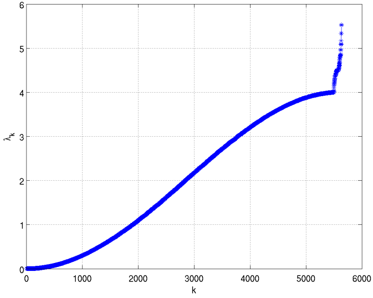

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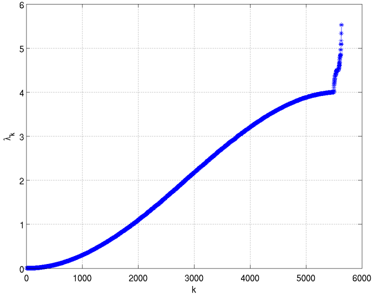

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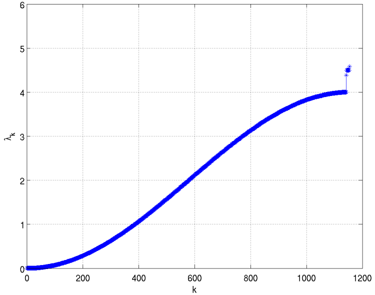

(b) RGC #100

Our Observation . . .

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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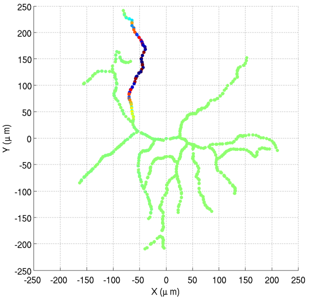

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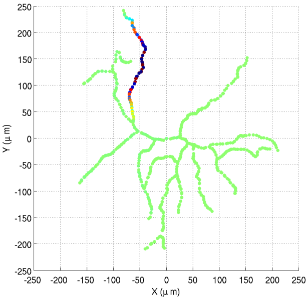

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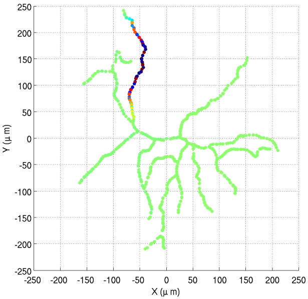

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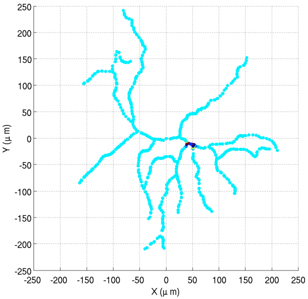

(b) RGC #100; $\lambda_{1142} = 4.3829$

Our Aim

We want to answer to the following questions:

- Why do such phase transitions in graph Laplacian eigenvalues and eigenfunctions occur in dendritic trees?
- Why the eigenvalue 4 is the threshold?
- What classes of graphs and trees reveal such a phenomenon?

Outline

Graph Laplacians

Let $G = (V, E)$ be a graph (in fact, a tree) representing a given dendritic tree, with the vertex set $V = V(G) = \{v_1, \dots, v_n\}$ where v_i represents the 3D coordinate of the ith sampled point of the dendritic tree, and the edge set $E = E(G) = \{e_1, \dots, e_{n-1}\}$ where e_k represents an edge (or line segment) connecting between adjacent vertices. Let $d(v_k) = d_{v_k}$ be the degree of the vertex v_k.

The Laplacian matrix (often called the combinatorial Laplacian matrix) of a graph $G = (V, E)$ is defined as

$$
\begin{aligned}
L(G) &:= D(G) - A(G) \\
D(G) &:= \mathrm{diag}(d_{v_1}, \dots, d_{v_n}) \quad \text{the degree matrix} \\
A(G) &= (a_{ij}) \quad \text{the adjacency matrix where} \\
a_{ij} &:= \begin{cases} 1 & \text{if } v_i \sim v_j; \\ 0 & \text{otherwise.} \end{cases}
\end{aligned}
$$

Graph Laplacians . . .

- Let $|V(G)| = n$, and let $0 = \lambda_0(G) \le \lambda_1(G) \le \cdots \le \lambda_{n-1}(G)$ be the sorted eigenvalues of $L(G)$.
- $m_G(\lambda) :=$ the multiplicity of λ.
- Let $I \subset \mathbb{R}$ be an interval of the real line. Then define $m_G(I) := \#\{\lambda_k(G) \in I\}$.
- Let $f \in L^2(V)$. Then $L(G)f(u) = d_u f(u) - \sum_{v \sim u} f(v)$, i.e., this is a generalization of the finite difference approximation to the Laplacian.
- After all, *sines* (*cosines*) are the eigenfunctions of the Laplacian on the *rectangular* domain with Dirichlet (Neumann) boundary condition. Moreover, many special functions, e.g., *spherical harmonics* and *Bessel functions* are part of the Laplacian eigenfunctions for the *spherical* and *cylindrical*,domains, respectively.
- Hence, the eigenfunction expansion of data measured at the vertices using the graph Laplacian eigenfunctions corresponds to Fourier (or spectral) analysis of the data on that graph.

Graph Laplacians . . .

- Furthermore, the eigenvalues of $L(G)$ reflect various intrinsic geometric and topological information about the graph including
  - connectivity or the number of separated components
  - diameter (the maximum distance over all pairs of vertices)
  - mean distance, . . .
  - Fan Chung: *Spectral Graph Theory*, AMS, 1997

    is an intertwined tale of eigenvalues and their use in unlocking a thousand secrets about graphs.

- However, eigenvalues of $L(G)$ cannot uniquely determine the graph G. $\rightsquigarrow$ Kac (1966): "Can one hear the shape of a drum?" $\Longrightarrow$ Gordon, Webb, & Wolpert (1992): "One cannot hear the shape of a drum."
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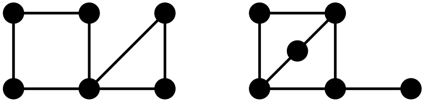

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- $\exists$ some attempts to reconstruct graphs from their Laplacian spectra via combinatorial optimization (e.g., Comellas & Diaz-Lopez, 2008)
- Nothing prevents us from using the Laplacian spectra for characterizing dendrite patterns!

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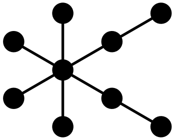

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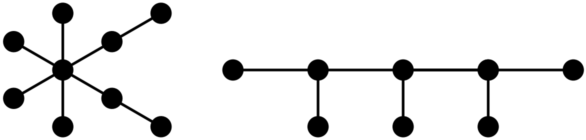

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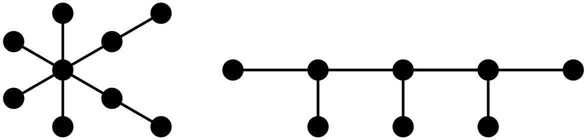

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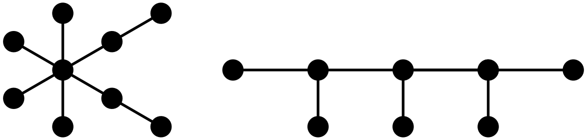

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A Simple Yet Important Example: A Path Graph

$$L(G) = D(G) - A(G)$$

$$\begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & & & & & \\ & 2 & & & & \\ & & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & \\ & & & & & 1 \end{bmatrix} - \begin{bmatrix} 0 & 1 & & & & \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & 0 & 1 \\ & & & & 1 & 0 \end{bmatrix}$$

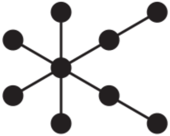
The eigenvectors of this matrix are exactly the DCT Type II basis vectors used for the JPEG image compression standard! (See e.g., Strang, SIAM Review, 1999).

- $\lambda_k = 2 - 2\cos(\pi k/n) = 4\sin^2(\pi k/2n),\ k = 0, 1, \ldots, n-1.$
- $\phi_k = \left(\cos(\pi k(\ell + \frac{1}{2})/n)\right)_{0 \le \ell < n},\ k = 0, 1, \ldots, n-1.$

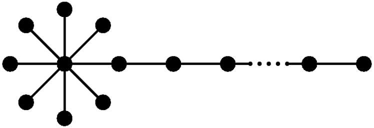
Outline

is a tree where there is only one vertex whose degree is larger than 2. We analyze this class of trees first because the real dendritic trees are more complicated.

- Let $S(n_1, n_2, \dots, n_k)$ 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: $n = 1 + \sum_{i=1}^{k} n_i$.



(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. However, we found that more general results had been already proven.
- 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 Own New Results on Starlike Trees

Corollary (S-W 2011)

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-W 2011, N-S-W 2011)

Let $\phi_{n-1} = (\phi_{1,n-1}, \cdots, \phi_{n,n-1})^{\mathrm{T}}$, 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.,

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

Why Is the Eigenvalue 4 Critical on Starlike Trees?

- 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 determinant of the characteristic equation is

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

- 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.

Outline

Our Observation via Numerical Experiments

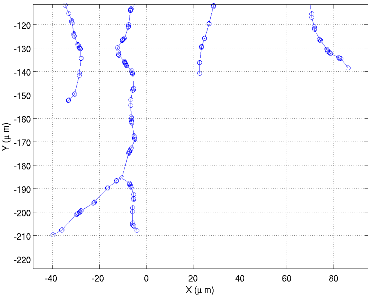
- Unfortunately, actual dendritic trees are not starlike.
- However, our numerical computations and data analysis indicate that:

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

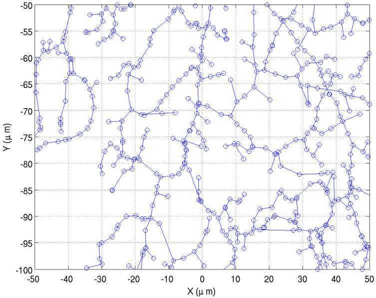
  for each cell where $n = |V(G)|$.
- We can define the starlikeliness $S\ell(T)$ of a given tree $G = T$ as follows:

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

Zoom Up of Some RGCs



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



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

Our Observation and Questions

Theorem (N-S-W 2011)

For any tree T of finite volume, we have

$$0 \le m_T([4,\infty)) \le \#\{j \in (1,n) \mid d(v_j) \gneqq 2\}$$

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

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Questions

- Is there any tree whose graph Laplacian has an exact eigenvalue 4?
- If so, what kind of trees are they?
- How about simple connected graphs instead of trees?

Our Conjecture and Questions . . .

- It turned out that Guo proved the following theorem:

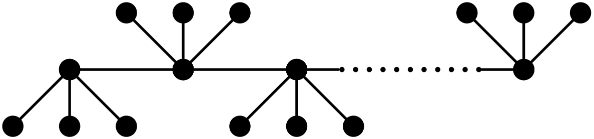
Theorem (Guo 2006)

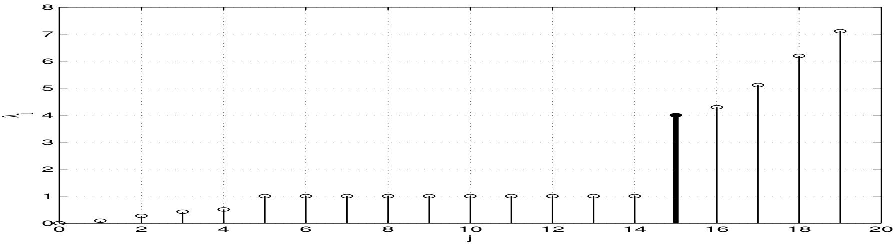
Let T be a tree with n vertices. Then,

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

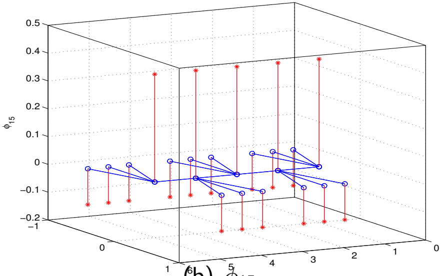
and the equality holds iff a) $j \neq 0$; b) $n-j$ divides n; and c) T is spanned by $n-j$ vertex disjoint copies of $K_{1,\frac{j}{n-j}}$.

- This implies that if $n = 4m$, there is an eigenvalue exactly equal to 4 at $j = 3m$, i.e., $\lambda_{3m} = 4$, and this tree consists of m copies of $K_{1,3}$:

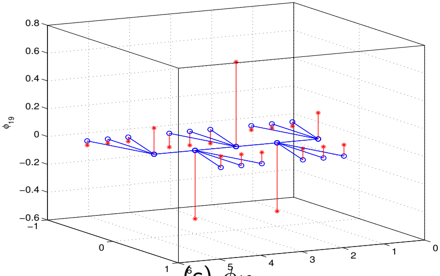




(a) $\{\lambda_j\}_{j=0}^{19}$; $S\ell(T) = 1$



(b) ϕ_{15}



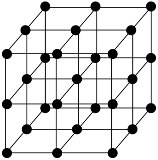
(c) ϕ_{19}

Can a simple connected graph have the exact eigenvalue 4?

- The answer is clear 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

$$\begin{aligned} \lambda_{j_1,\ldots,j_d} &= 4 \sum_{i=1}^{d} \sin^2 \left(\frac{j_i \pi}{2n} \right) \\ \phi_{j_1,\ldots,j_d}(x_1, \ldots, x_d) &= \prod_{i=1}^{d} \cos \left(\frac{j_i \pi (x_i + \frac{1}{2})}{n} \right), \end{aligned}$$

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.



- 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:

$$\boxed{\sum_{i=1}^{d} \sin^2\left(\frac{j_i \pi}{2n}\right) = 1.}$$

- For $d = 2$, it is easy to show that $m_G(4) = n - 1$.
- For $d = 3$, $m_G(4)$ behaves in a much more complicated manner, which is deeply related to number theory.
- We expect that more complicated situations occur for $d > 3$.

Outline

Summary

- We completely understood why the eigenvalue 4 plays a role of threshold for the phase transition phenomenon for starlike trees.
- We proved that the eigenfunction corresponding to the largest eigenvalue (≥ 4) reveals the concentration/localization phenomenon for starlike trees.
- For more general trees, the above statements are yet to be proved.
- However, we proved that the number of the eigenvalues greater than or equal to 4 is bounded from above by the number of vertices whose degree is larger than 2 for any tree.
- We also identified the unique class of trees (i.e., concatenations of claws) whose members have the exact eigenvalue 4.
- We also showed that there exist many graphs (not trees) that have the exact eigenvalue 4 (e.g., finite lattice graphs).
- A finite lattice graph with $d \geq 2$, have repeated eigenvalue 4 and the corresponding eigenfunctions reveal quite peculiar features; $\exists$ still many things to understand and prove!!

Outline

References, etc.

- Laplacian Eigenfunction Resource Page http://www.math.ucdavis.edu/~saito/lapeig/ contains
  - All the talk slides of the previous minisymposia "Laplacian Eigenfunctions and Their Applications, " which I co-organized for ICIAM 2007 (Zürich) and SIAM Imaging Conference 2008 (San Diego);
  - A Link to the recent workshop on "Laplacian eigenvalues and eigenfunctions: Theory, application, computation," Feb. 2009, at Institute for Pure and Applied Mathematics (IPAM), UCLA;
  - My Course Note (elementary) on "Laplacian Eigenfunctions: Theory, Applications, and Computations."
- NS is co-organizing a minisymposium on "Harmonic Analysis on Graphs and Networks: Theory and Applications" at ICIAM 2011 (Vancouver, Canada). Please come to the afternoon session today!
- The following article is available at http://www.math.ucdavis.edu/~saito/publications/
  - N. Saito and E. Woei: "On the phase transition phenomenon of graph Laplacian eigenfunctions on trees," RIMS Kokyuroku, vol.1743, 2011.