MAT 280: Harmonic Analysis on Graphs & Networks Lecture 5: Graph Laplacian Eigenvalues II

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Outline

Isoperimetric Number

Isospectrality; Spectral Characterization of Graphs

3 Applications to Morphological Feature Extraction from Dendritic Trees

- Motivation
- Eigenvalue-Based Features
- Conclusions & Future Plans

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• Let $S \subset V(G)$ be a nonempty subset of vertices of G.

• $\partial S := \{e = (u, v) \in E(G) \mid u \in S, v \notin S\}$, which is called the *boundary* of S.



 $S = \{\bullet\}, S^c = \{\circ\}$

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$$h(S) := \frac{|\partial S|}{\min\{|S|, |S^c|\}}.$$

- For the example graph in the previous page: |S| = 4; $|S^c| = 5$; $|\partial S| = 8$. Hence, h(S) = 8/4 = 2.
- The Cheeger ratio tells us the *quality of the cut* of V into S ∪ S^c: if S and S^c are well-balanced, i.e., |S| ≈ |S^c|, and ∃ few edges connecting S and S^c, then h(S) is small.
- The *isoperimetric number* (or a.k.a. the *Cheeger constant*) *i*(*G*) of *G* is defined as

$$i(G) := \inf_{S \subset V; S \neq \emptyset} \frac{|\partial S|}{\min\{|S|, |S^c|\}}.$$

- This definition is exactly the same as the one given in my previous lecture, but is in a more symmetric form.
- The version for L_{rw} replaces |S| and $|S^c|$ by vol(S) and $vol(S^c)$ where $vol(S) := \sum_{v \in S} d(v)$. That version has also been studied extensively.

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- To determine it, we need to find a small *edge-cut* separating as large a subset S with $|S| \le n/2$ as possible from the remaining larger part S^c. \implies It serves as a *measure of connectivity* of G. May indicate how easy is it to "destroy" a given network G by cutting only a few edges.

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 ⇒ It serves as a *measure of connectivity* of G. May indicate how easy is it to "destroy" a given network G by cutting only a few edges.
- The problem of partitioning V(G) into two equally sized subsets (to within one element) in such a way that the number of the edges in the cut is minimal, is known as the *bisection width* problem. There are many practical applications, e.g., VLSI design, etc.
- i(G): large \implies G has a large growth rate. More precisely, let $B_k(v)$ be the set of vertices of G at distance at most k from v, like a ball with center v and radius k. Then, $|B_{k+1}(v)|/|B_k(v)| \ge i(G)/d_{\max}(G)$.
- It is a discrete analogue of the *Cheeger constant* in Riemannian geometry, i.e., the minimal area of a hypersurface that divides a given compact Riemannian manifold into two disjoint pieces of equal volume.

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Isoperimetric Numbers of Specific Graphs

Graph G	Isoperimetric Number $i(G)$
Complete graph K_n	$i(K_n) = \lceil n/2 \rceil$
Path P_n	$i(P_n) = 1/\lfloor n/2 \rfloor$
Cycle C _n	$i(C_n) = 2/\lfloor n/2 \rfloor$
Bipartite complete graph $K_{p,q}$	$i(K_{p,q}) = \lceil pq/2 \rceil / \lfloor (p+q)/2 \rfloor$
Cube m -dimension Cb_m	$i(Cb_m) = 1$
Petersen Graph P	i(P) = 1

- Both are viewed as measures of connectivity of a given graph.
- While *i*(*G*) is more explicitly related to the connectivity of a graph than *a*(*G*), it is more difficult (i.e., combinatorial) to compute *i*(*G*) than *a*(*G*).
- Hence, the bounds of i(G) in terms of a(G) and the other quantities have been extensively studied.
- Mohar (1987, 1989): $a(G)/2 \le i(G) \le \sqrt{a(G)(2d_{\max}(G) a(G))}$ for $n \ge 4$, where $d_{\max}(G) := \max_j d_j$.

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Isospectrality

- The spectrum (i.e., the set of eigenvalues) $\Lambda(G)$ of L(G) cannot uniquely determine the graph G.
 - ~ Kac (1966): "Can one hear the shape of a drum?" ⇒ Gordon, Webb, & Wolpert (1992): "One cannot hear the shape of a drum."
 An example of "isospectral" graphs (Tan, 1998; Fujii & Katsuda, 1999):

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$$L(G_1) = \begin{bmatrix} 2 & -1 & 0 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 & 0 \\ 0 & -1 & 4 & -1 & -1 & -1 \\ 0 & 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & -1 & 2 & 0 \\ -1 & 0 & -1 & 0 & 0 & 2 \end{bmatrix} \neq L(G_2) = \begin{bmatrix} 2 & -1 & 0 & 0 & -1 & 0 \\ -1 & 3 & -1 & 0 & 0 & -1 \\ 0 & -1 & 3 & -1 & -1 & 0 \\ 0 & 0 & -1 & 1 & 0 & 0 \\ -1 & 0 & -1 & 0 & 3 & -1 \\ 0 & -1 & 0 & 0 & -1 & 2 \end{bmatrix}$$

But, $\Lambda(G_1) = \Lambda(G_2) = \{0, 0.7639, 2, 3, 3, 5.2361\}.$

- In fact, there are 58 pairs, 6 triples of isospectral graphs within all possible simple/undirected/unweighted graphs with n < 8 (Tan, 1998).
- However, certain classes of graphs can be completely determined by their Laplacian spectra: starlike trees (Omidi & Tajbakhsh, 2007), centipedes (Boulet, 2008),

- ∃ 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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Morphology of Network-like Structures





(b) Universe

Morphology of Retinal Ganglion Cells



Retinal Ganglion Cells (D. Hubel: Eye, Brain, & Vision, '95)


A Typical Neuron (from Wikipedia)

Structure of a Typical Neuron



- Neuroscientists' Objective: To understand how structural / morphological properties of dendritic trees of mouse retinal ganglion cells (RGCs) relate to the cell types and their functionality; how such properties change / evolve from newborn to adult
- Why mouse? \implies Great possibilities for genetic manipulation
- Data: 3D images of dendrites of RGCs via a confocal microscope
- State of the art: A manually intensive procedure using specialized software¹:
 - Trace and segment dendrite patterns from each 3D cube;
 - Extract geometric/morphological parameters (totally 14 parameters);
 - Apply a conventional bottom-up "hierarchical clustering" algorithm
- The extracted morphological parameters include: somal size; dendritic field size; total dendrite length; branch order; mean internal branch length; branch angle; mean terminal branch length, . . .
- It takes half a day per cell with a lot of human interactions!

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Motivation

3D Data



Mouse's RGC as a Graph



Clustering using Features Derived by Neurolucida®



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Our Goal

- We want to develop algorithms for *automatic* morphological feature extraction and clustering from such dendritic trees.
- To do so, we need to convert each dendritic tree to a feature vector in ℝ^k with relatively small k ∈ N. This is called a graph embedding into a vector space.
- In this lecture, we mainly consider the features using *eigenvalues of* graph Laplacians of such trees.

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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
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- n = |V(G)| ranges between 565 and 24474 depending on the RGCs.
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Outline

Isoperimetric Number

Isospectrality; Spectral Characterization of Graphs

3 Applications to Morphological Feature Extraction from Dendritic Trees

- Motivation
- Eigenvalue-Based Features
- Conclusions & Future Plans

Feature 1: $(p(G) - m_G(1))/|V(G)|$ as a lower bound of the number of pendant neighbors q(G) normalized by n = |V(G)|;

Feature 2: The normalized Wiener index W(G)/|V(G)|;

- Feature 3: $m_G(4,\infty)/|V(G)|$, i.e., the number of eigenvalues of L(G)larger than 4 (normalized);
- Feature 4: $\sqrt{a(G)(2\max_{v \in V(G)} d_v a(G))}$, i.e., the upper bound of the isoperimetric number i(G).
- We normalized Features 1, 2, 3, by n = |V(G)| because we wanted to make features less dependent on the number of samples or how the dendrite arbors are sampled. Of course, the number of vertices itself could be a feature although it may not be a decisive one.
- Feature 4 was not explicitly normalized because the isoperimetric number *i*(*G*) itself is a normalized quantity in terms of number of vertices.

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(a) RGC #60; F_1 large

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- 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;
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(a) RGC #100; λ₁₁₄₁ = 3.9994

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Recap: Clustering using Features Derived by Neurolucida®



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Results: Scatter Plot; Feature 1 vs Feature 2



Figure: A scatter plot of the normalized lower bounds of the number of the pendant neighbors vs the normalized Wiener indices.

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Graph Laplacian Eigenvalues II

Results: Scatter Plot; Feature 3 vs Feature 4



Figure: A scatter plot of the normalized number of the eigenvalues larger than 4 vs the upper bounds of the isoperimetric numbers.

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Graph Laplacian Eigenvalues II

Interpretation of the Results

- Cluster 6 RGCs separate themselves quite well from the other RGC clusters.
- In fact, the sparse and distributed dendrite patterns such as those in Clusters 6 and 10 are located below the major axis of the point clouds in the $F_1 - F_2$ scatter plot and above the major axis of the point clouds in the $F_3 - F_4$ scatter plot. \implies the dendrite patterns belonging to Cluster 6 and 10 have smaller number of spines and smaller Wiener indices compared to the other denser dendrite patterns such as Clusters 1 to 5
- Considerable feature variability in Clusters 7 and 8.

Cluster 1 vs Cluster 6 . . .



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Conclusions & Future Plans

- Network-like structures are abundant and need to be quantitatively analyzed.
- How to embed such graphs/networks into a vector space becomes important.
- Demonstrated the usefulness of the eigenvalues of graph Laplacians for dendrite pattern analysis although the results are still preliminary.
- Need to investigate more eigenvalue-based features.
- Need to investigate resampling of dendrite arbor samples.
- How about the weighted graph Laplacians?
- Analyze the features derived by Neurolucida[®]: are they derivable from the Laplacian eigenvalues?
- Automating segmentation of dendritic trees from 3D images will be highly useful although it is quite tough.