MAT 280: Harmonic Analysis on Graphs & Networks
Lecture 17: Wavelets on Graphs II
Organizing 'Dual' Domains of Graphs (Part 1)

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Outline

Acknowledgment

- Qinglan Xia (UC Davis)
- NSF Grants: DMS-1418779, IIS-1631329, DMS-1912747, CCF-1934568
- ONR Grants: N00014-16-1-2255

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Motivations

- Using graph Laplacian eigenvectors as "cosines" or Fourier modes on graphs with eigenvalues as (the square of) their "frequencies" has been quite popular.
- However, the notion of *frequency* is ill-defined on general graphs and the Fourier transform is not properly defined on graphs
- Graph Laplacian eigenvectors may also exhibit peculiar behaviors depending on *topology* and *structure* of given graphs!
- Spectral Graph Wavelet Transform (SGWT) of Hammond et al. derived wavelets on a graph based on *the Littlewood-Paley theory* that organized the graph Laplacian eigenvectors corresponding to dyadic partitions of eigenvalues by viewing the eigenvalues as "frequencies"
- Unfortunately, this view is wrong other than very simple graphs, e.g., undirected unweighted paths and cycles.

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A Simple Yet Important Example: A Path Graph

$$\underbrace{\begin{bmatrix} 1 & -1 & & & & \\ -1 & 2 & -1 & & & \\ & -1 & 2 & -1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & -1 & 2 & -1 \\ & & & & -1 & 1 \end{bmatrix}}_{L(G)} = \underbrace{\begin{bmatrix} 1 & & & & & \\ & 2 & & & & \\ & & 2 & & & \\ & & & \ddots & & \\ & & & & 2 & \\ & & & & & 1 \end{bmatrix}}_{D(G)} - \underbrace{\begin{bmatrix} 0 & 1 & & & & \\ 1 & 0 & 1 & & & \\ & 1 & 0 & 1 & & \\ & & \ddots & \ddots & \ddots & \\ & & & 1 & 0 & 1 \\ & & & & 1 & 0 \end{bmatrix}}_{W(G)}$$

The eigenvectors of this matrix are exactly the *DCT Type II* basis vectors (used for the JPEG standard) while those of the *symmetrically-normalized Graph Laplacian matrix* $L_{\mathrm{sym}} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$ are the *DCT Type I* basis! (See G. Strang, "The discrete cosine transform," *SIAM Review*, vol. 41, pp. 135–147, 1999).

- $\lambda_k = 2 - 2\cos(\pi k/n) = 4\sin^2(\pi k/2n),\ k = 0 : n-1.$
- $\boldsymbol{\phi}_k(\ell) = a_{k;n}\cos\left(\pi k\left(\ell + \frac{1}{2}\right)/n\right),\ k,\ell = 0 : n-1;\ a_{k;n}$ is a const. s.t. $\|\boldsymbol{\phi}_k\|_2 = 1.$
- In this simple case, λ (eigenvalue) is a monotonic function w.r.t. the frequency, which is the eigenvalue index k. *For a general graph, however, the notion of frequency is not well defined.*

Problem with 2D Lattice Graph

- As soon as the domain becomes *even slightly more complicated than* unweighted and undirected paths/cylces, the situation completely changes: we cannot view the eigenvalues as a simple monotonic function of frequency anymore.
- For example, consider a thin strip in $\mathbb{R}^2$, and suppose that the domain is discretized as $P_m \times P_n$ $(m > n)$, whose Laplacian eigenpairs are:

$$\lambda_k = 4\left[\sin^2\left(\frac{\pi k_x}{2m}\right) + \sin^2\left(\frac{\pi k_y}{2n}\right)\right],$$

$$\phi_k(x,y) = a_{k_x;m} a_{k_y;n} \cos\left(\frac{\pi k_x}{m}\left(x + \frac{1}{2}\right)\right) \cos\left(\frac{\pi k_y}{n}\left(y + \frac{1}{2}\right)\right),$$

where $k = 0 : mn-1$; $k_x = 0 : m-1$; $k_y = 0 : n-1$; $x = 0 : m-1$; and $y = 0 : n-1$.

- As always, let $\{\lambda_k\}_{k=0:mn-1}$ be ordered in the nondecreasing manner. In this case, the smallest eigenvalue is still $\lambda_0 = \lambda_{(0,0)} = 0$, and the corresponding eigenvector is constant.

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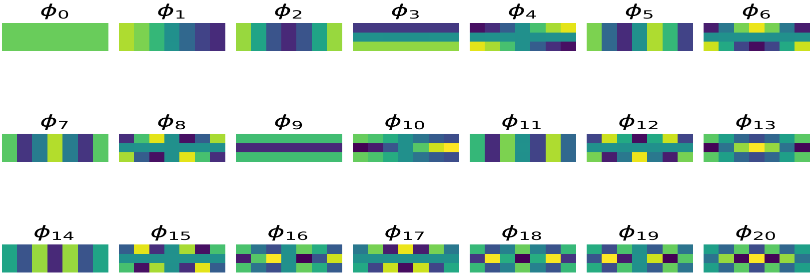
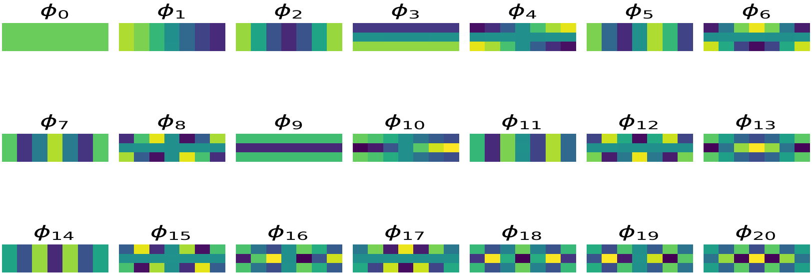


- The second smallest eigenvalue λ_1 is $\lambda_{(1,0)} = 4\sin^2(\pi/2m)$, since $\pi/2m < \pi/2n$, and its eigenvector has half oscillation in the x-direction.
- But, how about λ_2? Even for such a simple situation there are two possibilities: If $m > 2n$, then $\lambda_2 = \lambda_{(2,0)} < \lambda_{(0,1)}$. On the other hand, if $n < m < 2n$, then $\lambda_2 = \lambda_{(0,1)} < \lambda_{(2,0)}$.
- More generally, if $Kn < m < (K+1)n$ for some $K \in \mathbb{N}$, then $\lambda_k = \lambda_{(k,0)} = 4\sin^2(k\pi/2m)$ for $k = 0, \ldots, K$. Yet we have $\lambda_{K+1} = \lambda_{(0,1)} = 4\sin^2(\pi/2n)$ and λ_{K+2} is equal to either $\lambda_{(K+1,0)} = 4\sin^2((K+1)\pi/2m)$ or $\lambda_{(1,1)} = 4[\sin^2(\pi/2m) + \sin^2(\pi/2n)]$ depending on m and n.



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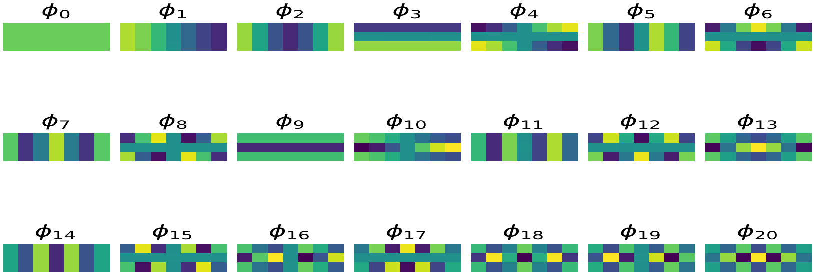

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- As one can see from this, the mapping between k and (k_x, k_y) is quite nontrivial. Notice that $\phi_{(k,0)}$ has $k/2$ oscillations in the x-direction whereas $\phi_{(0,1)}$ has only half oscillation in the y-direction.
- In other words, all of a sudden the eigenvalue of a completely different type of oscillation sneaks into the eigenvalue sequence.
- Hence, on a general domain or a general graph, by simply looking at the Laplacian eigenvalue sequence $\{\lambda_k\}_{k=0,1,\ldots}$, it is *almost impossible to organize the eigenpairs into physically meaningful dyadic blocks* and apply the Littlewood-Paley approach unless the underlying domain is of very simple nature, e.g., P_n or C_n.
- For complicated domains, the notion of *frequency* is not well-defined anymore, and thus wavelet construction methods that rely on the Littlewood-Paley theory by viewing eigenvalues as the square of frequencies, such as the spectral graph wavelet transform (SGWT) of Hammond et al. may lead to unexpected problems on general graphs.

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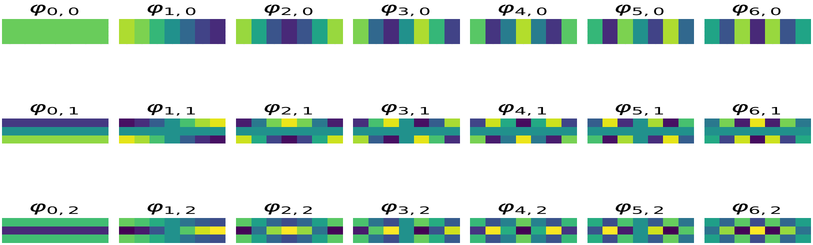
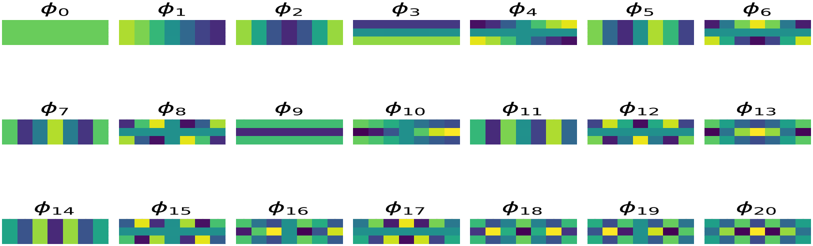
What we want to do is to *organize* those eigenvectors as



instead of



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Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\|\boldsymbol{\phi}_i - \boldsymbol{\phi}_j\right\|_2 = \sqrt{2}\delta_{i \neq j}$.
- Consider the *optimal transport theory*!
  - Convert each $\boldsymbol{\phi}_i$ to a probability mass function (pmf) $\boldsymbol{p}_i$ over a graph G (e.g., via squaring each component of $\boldsymbol{\phi}_i$)
  - Compute the cost to transport $\boldsymbol{p}_i$ to $\boldsymbol{p}_j$ optimally (a.k.a. *Earth Mover's Distance* or *1st Wasserstein Distance*), for all $i, j = 0 : n-1$, which results in a "distance" matrix $D \in \mathbb{R}^{n \times n}_{\geq 0}$
  - *Embed* the eigenvectors into a lower dimensional Euclidean space, say, $\mathbb{R}^m$, $m \ll n$ (typically $m = 2$ or $m = 3$) so that the distances among those embedded points match with those given in D (can use, e.g., *Multidimensional Scaling* (MDS))
  - *Organize* and *group* those points to *generate wavelet-like vectors on G*
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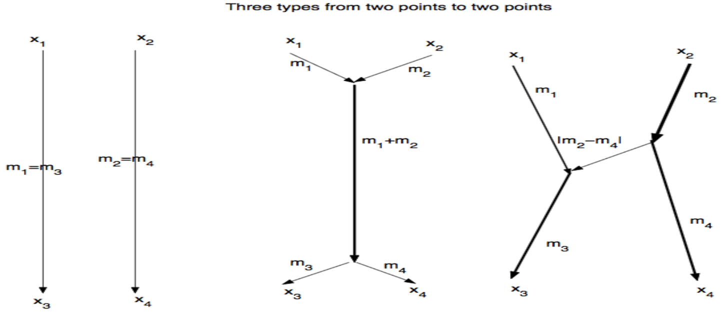

- is the study of *branching* structures, e.g., trees; veins on a leaf; cardiovascular systems; river channel networks; electrical grids; communication networks, etc.

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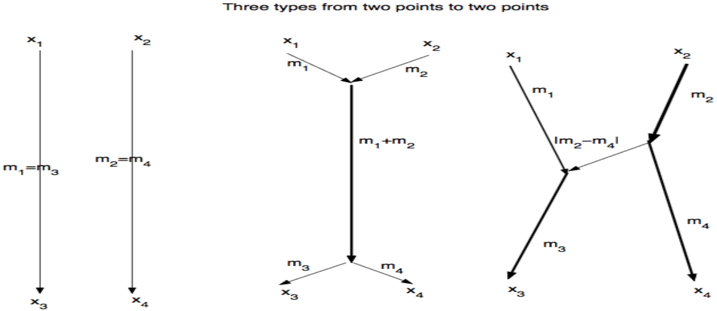

- is the study of *branching* structures, e.g., trees; veins on a leaf; cardiovascular systems; river channel networks; electrical grids; communication networks, etc.

ROT: Discrete Version

- Definitions: Two discrete mass distributions (a.k.a. atomic measures) in $\mathbb{R}^d$: $\boldsymbol{a} := \sum_{i=1}^{k} m_i \delta_{\boldsymbol{x}_i}$; $\boldsymbol{b} := \sum_{j=1}^{l} n_j \delta_{\boldsymbol{y}_j}$; $\{\boldsymbol{x}_i\}_i, \{\boldsymbol{y}_j\}_j \subset \mathbb{R}^d$; $\sum_{i=1}^{k} m_i = \sum_{j=1}^{l} n_j$.
- Let $\mathrm{Path}(\boldsymbol{a}, \boldsymbol{b})$ be all possible transport paths from $\boldsymbol{a}$ to $\boldsymbol{b}$ without cycles (Xia could manage to remove cycles), i.e., each $G \in \mathrm{Path}(\boldsymbol{a}, \boldsymbol{b})$ is a weighted acyclic directed graph with $\{\boldsymbol{x}_i\}_i \cup \{\boldsymbol{y}_j\}_j \subset V(G)$, whose edge weights (>0) satisfy *the Kirchhoff law* at each interior node $v \in V(G) \setminus \{\boldsymbol{x}_i, \boldsymbol{y}_j\}_{i,j}$:

$$\sum_{e \in E(G); e^- = v} w(e) = \sum_{e \in E(G); e^+ = v} w(e) + \begin{cases} m_i & \text{if } v = \boldsymbol{x}_i \text{ for some } i \in 1:k \\ -n_j & \text{if } v = \boldsymbol{y}_j \text{ for some } j \in 1:l \\ 0 & \text{otherwise.} \end{cases}$$

- Define the cost of a transport path $G \in \mathrm{Path}(\boldsymbol{a}, \boldsymbol{b})$:

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Xia further derived:

- Number of branching nodes in $\mathrm{Path}(\boldsymbol{a}, \boldsymbol{b})$ can be bounded from above by $k + l - 2$.
- The uniform lower bounds of minimum angle between any two edges in any α-optimal path in $\mathrm{Path}(\boldsymbol{a}, \boldsymbol{b})$.
- The minimum transportation cost $d_\alpha(\boldsymbol{a}, \boldsymbol{b}) := \min_{G \in \mathrm{Path}(\boldsymbol{a}, \boldsymbol{b})} \boldsymbol{M}_\alpha(G)$ is a *metric* on the space of atomic measures of equal mass and is of homogeneous of degree α, i.e., $d_\alpha(\lambda \boldsymbol{a}, \lambda \boldsymbol{b}) = \lambda^\alpha d_\alpha(\boldsymbol{a}, \boldsymbol{b})$, $\forall \lambda > 0$.
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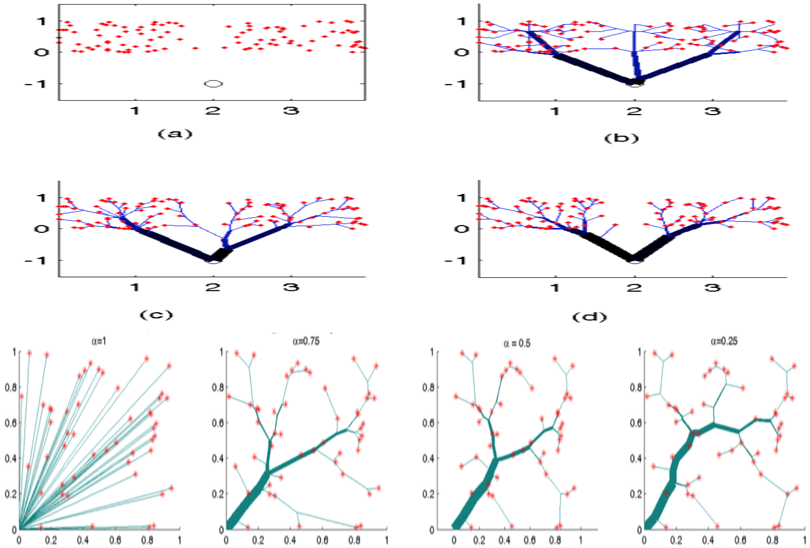
ROT: Numerical Examples



Our Method to Compute Transportation Costs

- Unlike the general ROT setting, a graph G is fixed and given.
- In general, we want to deal with *undirected* graphs.
- The ROT only deals with *directed* graphs.
- Hence, we turn an undirected graph G into the *bidirected* graph $\tilde{\tilde{G}}$.
- To do so, we first compute the *incidence matrix* $Q = [\boldsymbol{q}_1|\cdots|\boldsymbol{q}_m] \in \mathbb{R}^{n\times m}$ of the undirected graph $G = G(V,E)$ with $n = |V|$, $m = |E|$. Here, $\boldsymbol{q}_k$ represents the endpoints of e_k: if e_k joins nodes i and j, then $\boldsymbol{q}_k[l] = 1$ if $l = i$ or $l = j$; otherwise $\boldsymbol{q}_k[l] = 0$.
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$$\tilde{\boldsymbol{q}}_k[l] = \begin{cases} -1 & \text{if } l = i; \\ 1 & \text{if } l = j; \\ 0 & \text{otherwise.} \end{cases}$$

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- Given $\tilde{\tilde{Q}}$, we solve the *balance equation* that forces the Kirchhoff law:

$$\tilde{\tilde{Q}}\boldsymbol{w}_{ij} = \boldsymbol{p}_j - \boldsymbol{p}_i, \quad \boldsymbol{w}_{ij} \in \mathbb{R}^{2m}_{\geq 0}. \qquad (*)$$

- The weight vector $\boldsymbol{w}_{ij}$ describes the transportation plan of mass from $\boldsymbol{p}_i$ to $\boldsymbol{p}_j$, i.e., let $\tilde{\tilde{G}}_{ij}$ be the bidirected graph $\tilde{\tilde{G}}$ with these edge weights; then $\tilde{\tilde{G}}_{ij} \in \mathrm{Path}(\boldsymbol{p}_i, \boldsymbol{p}_j)$.
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- Currently, we use the following *Linear Programming* (LP):

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  to obtain one of the *sparse* solutions of Eqn. $(*)$, which turned out to be better than using nonnegative least squares (NNLS) solver.

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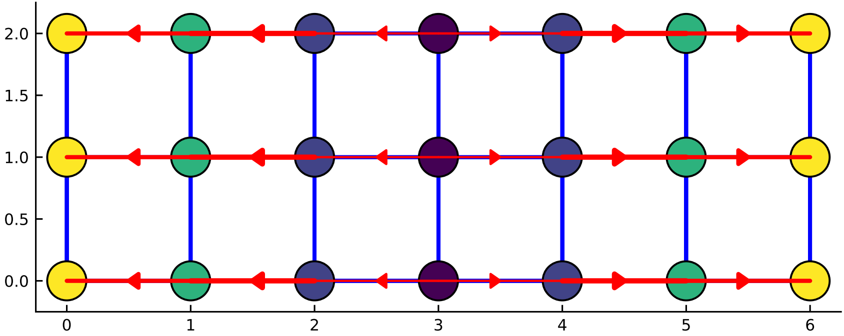
Outline

2D Regular Lattice: An LP Solution to ($*$)

Consolidated $\boldsymbol{w}_{0,1}$: mass transport from $\boldsymbol{p}_0 = \boldsymbol{\phi}_0^2$ to $\boldsymbol{p}_1 = \boldsymbol{\phi}_1^2$



2D Regular Lattice: An NNLS Solution to $(*)$

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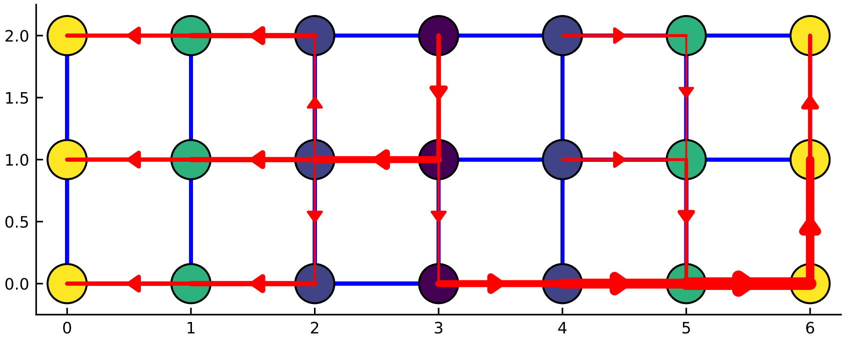
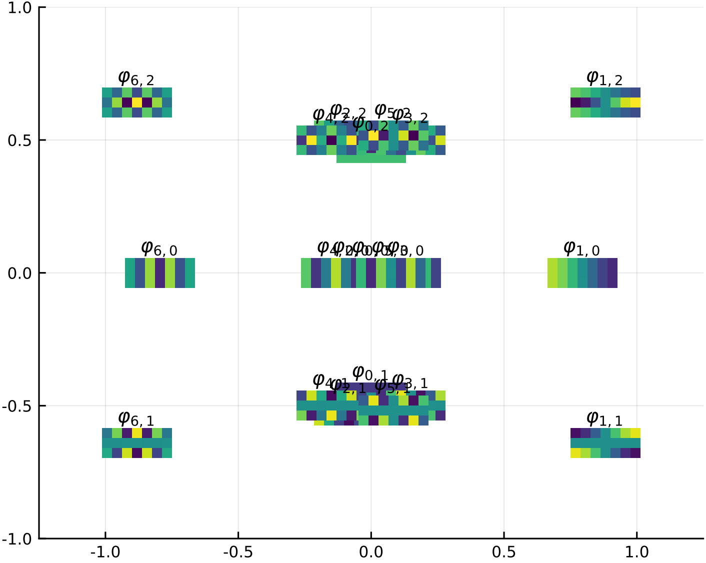


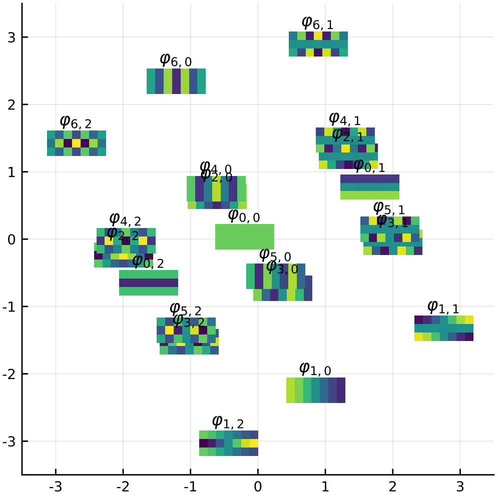
2D Regular Lattice: Embedding into $\mathbb{R}^2$; $\alpha = 1$



2D Regular Lattice: Embedding into $\mathbb{R}^2$; $\alpha = 0.5$

Some symmetry could be explained because of the symmetry of DCT vectors:

$$\phi^2_{k;n}[x] + \phi^2_{n-k;n}[x] \equiv a^2_{k;n} = 2/n, \; k = 1:n-1, \; x = 0:n-1.$$



Other Ways to Turn $\boldsymbol{\phi}_i$ into $\boldsymbol{p}_i$

- Generating $\boldsymbol{\phi}_i^2$ is not the only way to turn $\boldsymbol{\phi}_i$ into a pmf $\boldsymbol{p}_i$.
- Other examples include:
  - Normalized ℓ^1: $\boldsymbol{\phi}_i^1 := \left(|\phi_i[0]|, \ldots, |\phi_i[n-1]|\right)^{\mathsf{T}} / \|\boldsymbol{\phi}_i\|_1$;
  - A constant addition followed by normalization:

$$\tilde{\boldsymbol{\phi}}_i := \begin{cases} \boldsymbol{\phi}_0^1 & \text{if } i = 0; \\ \dfrac{\boldsymbol{\phi}_i - c_{\min} \cdot \mathbf{1}_n}{\|\boldsymbol{\phi}_i - c_{\min} \cdot \mathbf{1}_n\|_1} & \text{if } i \neq 0, \end{cases}$$

    where $c_{\min} := \min_{0<i<n;\, 0\le l<n} \phi_i[l] < 0$;
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- Generating $\boldsymbol{\phi}_i^2$ is not the only way to turn $\boldsymbol{\phi}_i$ into a pmf $\boldsymbol{p}_i$.
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$$\widetilde{\boldsymbol{\phi}}_i := \begin{cases} \boldsymbol{\phi}_0^1 & \text{if } i = 0; \\ \frac{\boldsymbol{\phi}_i - c_{\min} \cdot \mathbf{1}_n}{\|\boldsymbol{\phi}_i - c_{\min} \cdot \mathbf{1}_n\|_1} & \text{if } i \neq 0, \end{cases}$$

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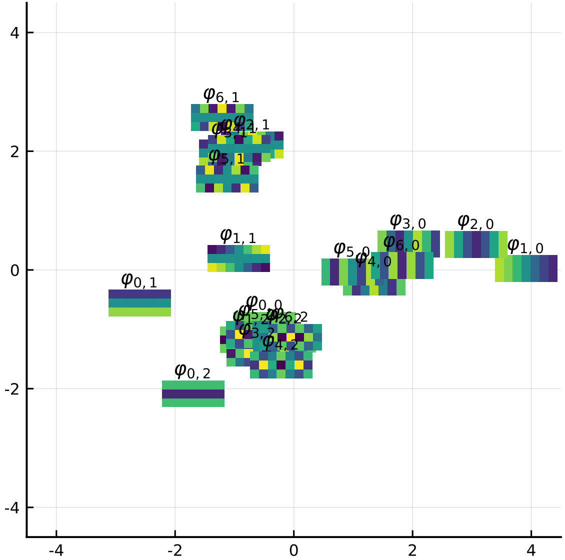
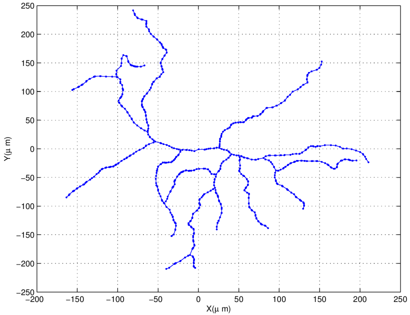
2D Regular Lattice; via $\{\boldsymbol{\phi}_i^{\mathrm{e}}\}_i$, $\alpha = 0.25$



Outline

A Peculiar Phase Transition Phenomenon

We observed an interesting phase transition phenomenon on the behavior of the eigenvalues of *graph Laplacians* defined on dendritic trees.



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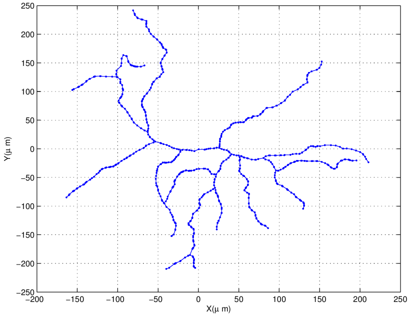

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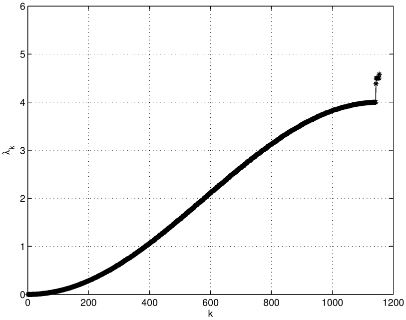

(b) Eigenvalues of RGC #100

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;
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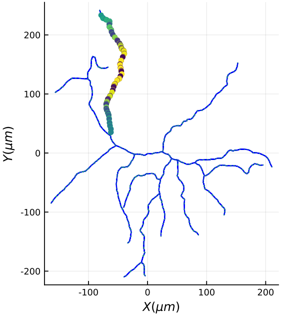

(a) RGC #100; $\lambda_{1141} = 3.9994$

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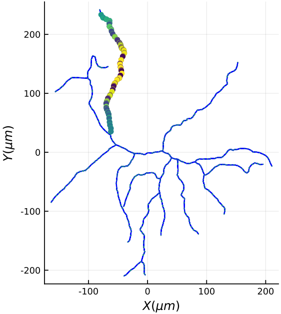

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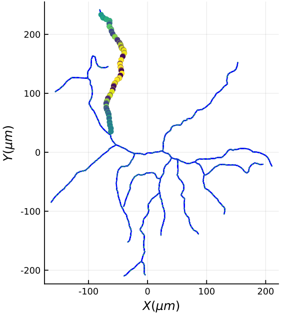

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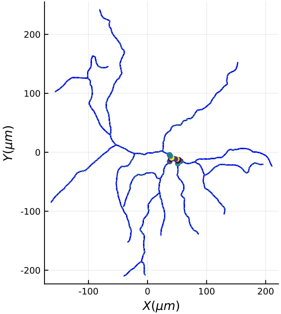

(b) RGC #100; $\lambda_{1142} = 4.3829$

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- Any physiological consequence? Importance of branching vertices?
- Many such eigenvector localization phenomena have been reported: Anderson localization, scars in quantum chaos, ...
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- Our point is that eigenvectors, especially those corresponding to high eigenvalues, are quite sensitive to *topology and geometry of the underlying domain* and cannot really be viewed as high frequency oscillations unless the underlying graph is a simple unweighted path or cycle.
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Embedding of Eigenvectors on the Dendritic Tree into $\mathbb{R}^3$

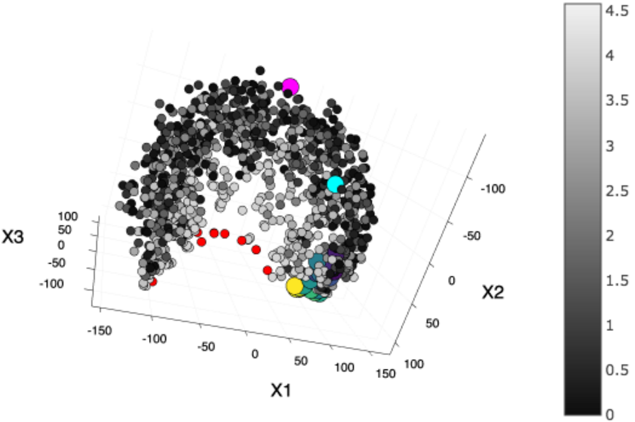
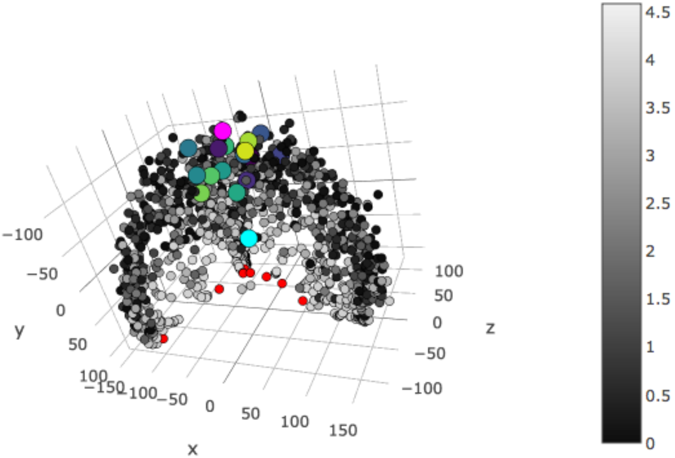


Figure: The magenta circle = the DC vector; the cyan circle = the Fiedler vector; the red circles = the localized eigenvectors; the larger colored circles = the eigenvectors supported on the upper-left branch



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Outline

References

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- N. Saito: "How can we naturally order and organize graph Laplacian eigenvectors?" in *Proc. 2018 IEEE Workshop on Statistical Signal Processing*, pp. 483–487, 2018. Also arXiv: 1801.06782 [math.SP].