Graph Wavelets via Natural Organization of Laplacian Eigenvectors

Naoki Saito
in collaboration with
Haotian Li (UCD) and Alex Cloninger (UCSD)

Department of Mathematics
University of California, Davis

Minisymposium on *Distance Metrics and Mass Transfer Between High Dimensional Point Clouds*
The 9th International Congress on Industrial and Applied Mathematics
Valencia, Spain, July 17, 2019

Outline

1. Motivations
2. Measuring Differences between Eigenvectors
3. Numerical Experiments
4. Organizing Laplacian Eigenvectors of Dendritic Trees
5. Other Methods for Eigenvector Organization
6. Building Natural Graph Wavelets
7. Summary

Acknowledgment

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

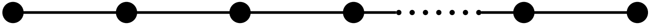
Outline

1. Motivations
2. Measuring Differences between Eigenvectors
3. Numerical Experiments
4. Organizing Laplacian Eigenvectors of Dendritic Trees
5. Other Methods for Eigenvector Organization
6. Building Natural Graph Wavelets
7. Summary

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 may face difficulty for graphs more complicated than very simple undirected unweighted paths and cycles.

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* $L_{\text{sym}} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$ 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

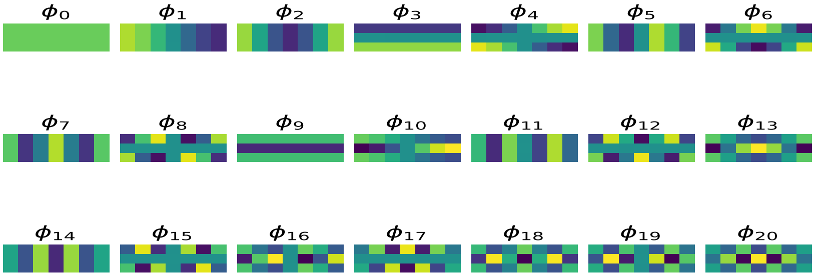
- As soon as the domain becomes *even slightly more complicated than* unweighted and undirected paths/cycles, the situation completely changes: *we cannot view the eigenvalues as a simple monotonic function of frequency anymore.*
- For example, consider a thin strip in $\mathbb{R}^2$, and suppose that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

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

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

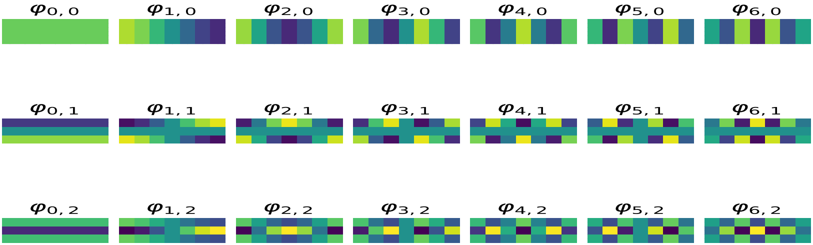
where $k = 0 : mn-1$; $k_x = 0 : m-1$; $k_y = 0 : n-1$; $x = 0 : m-1$; and $y = 0 : n-1$.

- 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.

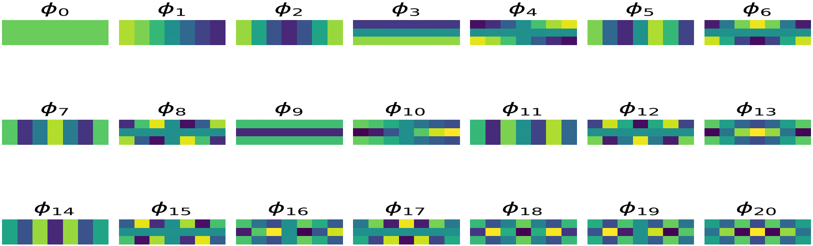


- All of a sudden the eigenvalue of a completely different type of oscillation sneaks into the eigenvalue sequence.
- Hence, on a general domain or a general graph, by simply looking at the Laplacian eigenvalue sequence $\{\lambda_k\}_{k=0,1,\ldots}$, it is *almost impossible to organize the eigenpairs 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.

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


$\varphi_{0,0}$ $\varphi_{1,0}$ $\varphi_{2,0}$ $\varphi_{3,0}$ $\varphi_{4,0}$ $\varphi_{5,0}$ $\varphi_{6,0}$
$\varphi_{0,1}$ $\varphi_{1,1}$ $\varphi_{2,1}$ $\varphi_{3,1}$ $\varphi_{4,1}$ $\varphi_{5,1}$ $\varphi_{6,1}$
$\varphi_{0,2}$ $\varphi_{1,2}$ $\varphi_{2,2}$ $\varphi_{3,2}$ $\varphi_{4,2}$ $\varphi_{5,2}$ $\varphi_{6,2}$

instead of


ϕ_0 ϕ_1 ϕ_2 ϕ_3 ϕ_4 ϕ_5 ϕ_6
ϕ_7 ϕ_8 ϕ_9 ϕ_{10} ϕ_{11} ϕ_{12} ϕ_{13}
ϕ_{14} ϕ_{15} ϕ_{16} ϕ_{17} ϕ_{18} ϕ_{19} ϕ_{20}

Outline

1. Motivations
2. Measuring Differences between Eigenvectors
3. Numerical Experiments
4. Organizing Laplacian Eigenvectors of Dendritic Trees
5. Other Methods for Eigenvector Organization
6. Building Natural Graph Wavelets
7. Summary

Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\| \boldsymbol{\phi}_i - \boldsymbol{\phi}_j \right\|_2 = \sqrt{2}\delta_{i \neq j}$.
- Enter 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 $D \in \mathbb{R}_{\geq 0}^{n \times n}$
  - *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*
- Can we get the "*dual geometry*" of G in that embedded space?

Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\|\boldsymbol{\phi}_i - \boldsymbol{\phi}_j\right\|_2 = \sqrt{2}\delta_{i\neq j}$.
- Enter 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*
- Can we get the "*dual geometry*" of G in that embedded space?

Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\|\boldsymbol{\phi}_i - \boldsymbol{\phi}_j\right\|_2 = \sqrt{2}\delta_{i\neq j}$.
- Enter 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*
- Can we get the "*dual geometry*" of G in that embedded space?

Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\|\boldsymbol{\phi}_i - \boldsymbol{\phi}_j\right\|_2 = \sqrt{2}\delta_{i \neq j}$.
- Enter 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 $D \in \mathbb{R}_{\geq 0}^{n \times n}$
  - *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*
- Can we get the "*dual geometry*" of G in that embedded space?

Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\|\boldsymbol{\phi}_i - \boldsymbol{\phi}_j\right\|_2 = \sqrt{2}\delta_{i \neq j}$.
- Enter 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*
- Can we get the "*dual geometry*" of G in that embedded space?

Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\|\boldsymbol{\phi}_i - \boldsymbol{\phi}_j\right\|_2 = \sqrt{2}\delta_{i \neq j}$.
- Enter 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 $D \in \mathbb{R}_{\geq 0}^{n \times n}$
  - *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*
- Can we get the "*dual geometry*" of G in that embedded space?

Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\|\boldsymbol{\phi}_i - \boldsymbol{\phi}_j\right\|_2 = \sqrt{2}\delta_{i \neq j}$.
- Enter 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*
- Can we get the "*dual geometry*" of G in that embedded space?

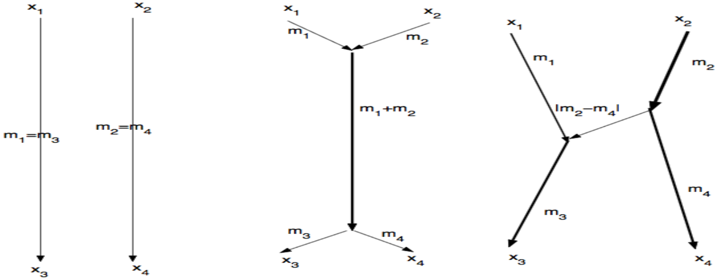
Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\| \boldsymbol{\phi}_i - \boldsymbol{\phi}_j \right\|_2 = \sqrt{2}\delta_{i \neq j}$.
- Enter 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*
- Can we get the "*dual geometry*" of G in that embedded space?

Ramified Optimal Transportation (ROT) by Q. Xia

- is the study of transporting "mass" from one Radon measure (or simply a probability measure) μ^+ to another μ^- along ramified transport paths with some specific transport cost functional.

Three types from two points to two points



- 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 (aka 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 $G \in \mathrm{Path}(\boldsymbol{a}, \boldsymbol{b})$:

$$\boldsymbol{M}_\alpha(G) := \sum_{e \in E(G)} w(e)^\alpha \,\mathrm{length}(e), \quad \alpha \in [0, 1].$$

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* $Q = \left[\boldsymbol{q}_1 | \cdots | \boldsymbol{q}_m\right] \in \mathbb{R}^{n \times m}$ 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 $\boldsymbol{q}_k[l] = 0$.
- Then orient the edges in $E(G)$ in an arbitrary manner to form a directed graph $\tilde{G}$ whose incidence matrix $\tilde{Q}$ is, e.g.,

$$\widetilde{\boldsymbol{q}}_k[l] = \begin{cases} -1 & \text{if } l = i; \\ 1 & \text{if } l = j; \\ 0 & \text{otherwise.} \end{cases}$$

- Finally, form the bidirected graph $\tilde{\tilde{G}}$ with $\tilde{\tilde{Q}} := \left[\tilde{Q} \mid -\tilde{Q}\right] \in \mathbb{R}^{n \times 2m}$.

Our Method to Compute Transportation Costs . . .

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

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

- 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 $\tilde{\tilde{G}}_{ij} \in \mathrm{Path}(\boldsymbol{p}_i, \boldsymbol{p}_j)$.
- Eqn. $(*)$ may have multiple solutions.

Our Method to Compute Transportation Costs . . .

- Currently, we use the following *Linear Programming* (LP):

  $$\min_{\boldsymbol{w}_{ij}\in\mathbb{R}^{2m}} \|\boldsymbol{w}_{ij}\|_1 \quad \text{subject to: } \tilde{\tilde{Q}}\boldsymbol{w}_{ij} = \boldsymbol{p}_j - \boldsymbol{p}_i; \boldsymbol{w}_{ij}[l] \geq 0, l = 0:(2m-1)$$

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

- Finally fill the distance matrix entries $D = (D_{ij})$:

  $$D_{ij} = \boldsymbol{M}_\alpha(\tilde{\tilde{G}}_{ij}) = \sum_{e\in E(\tilde{\tilde{G}}_{ij})} w_{ij}(e)^\alpha \,\mathrm{length}(e), \quad \alpha \in [0,1].$$

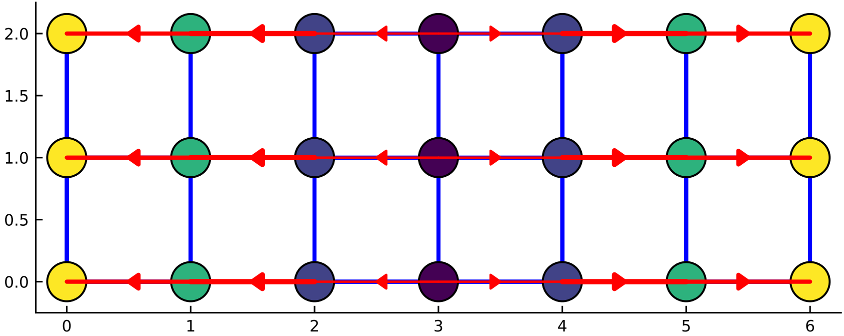
- Note that currently we are *not* examining all possible solutions of Eqn. $(*)$ to search $\arg \min_{\tilde{\tilde{G}}_{ij}\in\mathrm{Path}(\boldsymbol{p}_i,\boldsymbol{p}_j)} \boldsymbol{M}_\alpha(\tilde{\tilde{G}}_{ij})$.

Outline

1. Motivations
2. Measuring Differences between Eigenvectors
3. Numerical Experiments
4. Organizing Laplacian Eigenvectors of Dendritic Trees
5. Other Methods for Eigenvector Organization
6. Building Natural Graph Wavelets
7. Summary

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

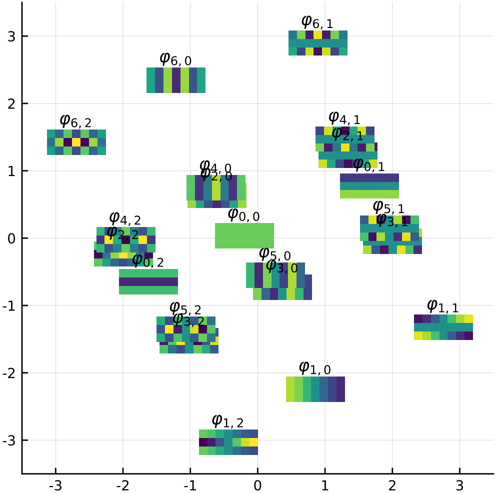
Consolidated $\boldsymbol{w}_{0,1}$: mass transport from $\boldsymbol{p}_0 = \boldsymbol{\phi}_0^2$ to $\boldsymbol{p}_1 = \boldsymbol{\phi}_1^2$



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

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

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



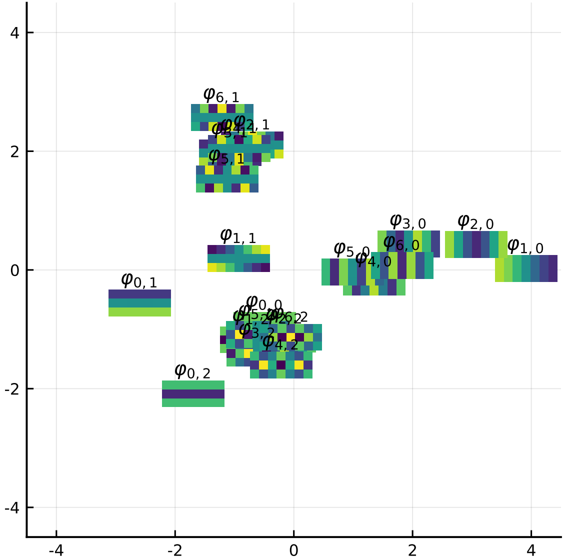
Other Ways to Turn $\boldsymbol{\phi}_i$ into $\boldsymbol{p}_i$

- 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: $\boldsymbol{\phi}_i^1 := \left(\left|\phi_i[0]\right|, \ldots, \left|\phi_i[n-1]\right|\right)^{\mathsf{T}} / \|\boldsymbol{\phi}_i\|_1$;
  - A constant addition followed by normalization:

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

    where $c_{\min} := \min_{0<i<n; 0 \le l < n} \phi_i[l] < 0$;
  - Normalized exponentiation: $\boldsymbol{\phi}_i^{\mathrm{e}} := \exp(\boldsymbol{\phi}_i) / \|\exp(\boldsymbol{\phi}_i)\|_1$.

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



Outline

1. Motivations

2. Measuring Differences between Eigenvectors

3. Numerical Experiments

4. Organizing Laplacian Eigenvectors of Dendritic Trees

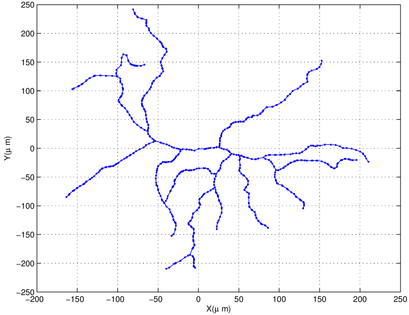
5. Other Methods for Eigenvector Organization

6. Building Natural Graph Wavelets

7. Summary

A Peculiar Phase Transition Phenomenon

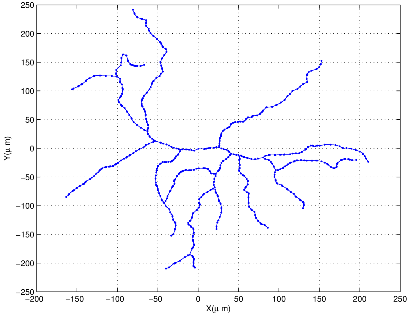
We observed an interesting phase transition phenomenon on the behavior of the eigenvalues of *graph Laplacians* defined on dendritic trees.



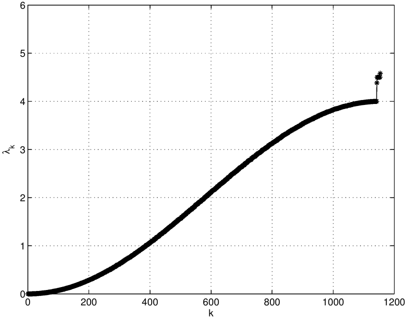
(a) RGC #100

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.



(a) RGC #100



(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;
- those corresponding to the eigenvalues above 4 are much more *localized* (like *wavelets*) around *junctions/bifurcation vertices*.

A Peculiar Phase Transition Phenomenon . . .

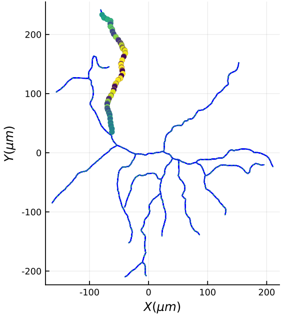
We have observed that this value 4 is critical since:

- 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*.

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*.

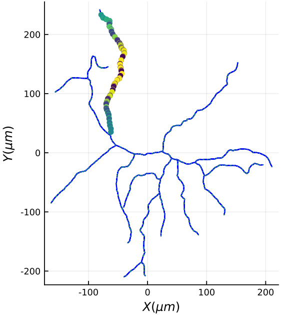


(a) RGC #100; $\lambda_{1141} = 3.9994$

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*.

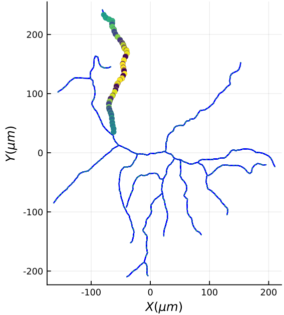


(a) RGC #100; $\lambda_{1141} = 3.9994$

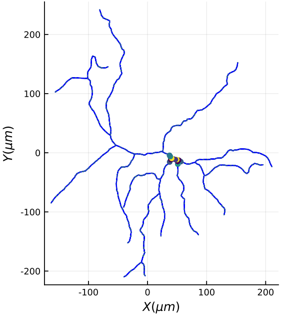
A Peculiar Phase Transition Phenomenon . . .

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*.



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



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

- We know why such localization/phase transition occurs $\Longrightarrow$ See our article for the detail: Y. Nakatsukasa, N. Saito, & E. Woei: "Mysteries around graph Laplacian eigenvalue 4," *Linear Algebra & Its Applications*, vol. 438, no. 8, pp. 3231–3246, 2013. The key was the *discriminant* of a quadratic equation.
- Many such eigenvector localization phenomena have been reported: Anderson localization, scars in quantum chaos, ...
- 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.
- Hence, one must be very careful to develop an analog of *the Littlewood-Paley theory* for general graphs!

Embedding of Eigenvectors on the Dendritic Tree into $\mathbb{R}^3$

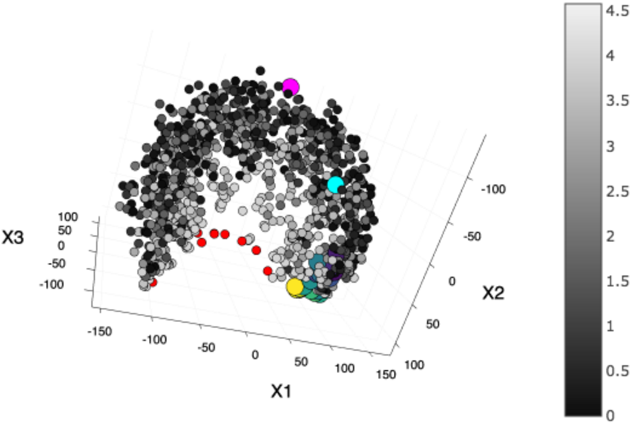


Figure: The magenta circle = the DC vector; the cyan circle = the Fiedler vector; the red circles = the localized eigenvectors; the larger colored circles = the eigenvectors supported on the upper-left branch

Outline

1. Motivations
2. Measuring Differences between Eigenvectors
3. Numerical Experiments
4. Organizing Laplacian Eigenvectors of Dendritic Trees
5. Other Methods for Eigenvector Organization
6. Building Natural Graph Wavelets
7. Summary

Various Methods for Eigenvector Organization

- A *similarity* measure based on the *average of local correlations* of eigenvectors (A. Cloninger & S. Steinerberger, 2018)
- The *difference of absolute gradient* (DAG) method (H. Li & N. Saito, 2019)
- The *time-stepping diffusion* (TSD) method (H. Li & N. Saito, 2019)
- For the details of the latter two, see our forthcoming paper (to be presented at *the SPIE Conference on Wavelets & Sparsity XVIII* in San Diego, CA, this August!)

Outline

1 Motivations

2 Measuring Differences between Eigenvectors

3 Numerical Experiments

4 Organizing Laplacian Eigenvectors of Dendritic Trees

5 Other Methods for Eigenvector Organization

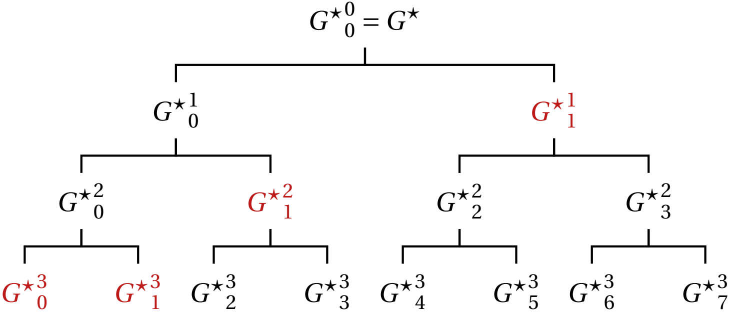
6 Building Natural Graph Wavelets

7 Summary

Natural Graph Wavelet Packet Dictionary

There may be a number of different ways to group and organize the graph Laplacian eigenvectors once the mutual distances are computed. Below, we discuss one of the simplest ones.

1. Given a graph $G = \{V, E, W\}$ with $|V| = n$ and the distance matrix $D = (D_{ij})$ of its eigenvectors, construct a *dual graph* $G^\star = \{V^\star, E^\star, W^\star\}$ where the ith node in $V^\star$ represents $\boldsymbol{\phi}_i$, and the edge weight $W^\star_{ij}$ reflects the affinity between $\boldsymbol{\phi}_i$ and $\boldsymbol{\phi}_j$, e.g., $W^\star_{ij} = 1/D_{ij}$ or $\exp(-D^2_{ij}/\sigma^2)$ for some appropriate scale parameter σ.
2. Construct a *hierarchical partition tree* of $G^\star$ using, e.g., the recursive bi-partition method that was used to construct our other graph wavelet packets such as the Hierarchical Graph Laplacian Eigen Transform (HGLET) and the Generalized Haar-Walsh Transform (GHWT). This corresponds to *hierarchical partitioning of the frequency domain in the conventional time-frequency analysis, which generates classical wavelet packets*.



$G^{\star 0}_{0} = G^{\star}$

$G^{\star 1}_{0}$ $G^{\star 1}_{1}$

$G^{\star 2}_{0}$ $G^{\star 2}_{1}$ $G^{\star 2}_{2}$ $G^{\star 2}_{3}$

$G^{\star 3}_{0}$ $G^{\star 3}_{1}$ $G^{\star 3}_{2}$ $G^{\star 3}_{3}$ $G^{\star 3}_{4}$ $G^{\star 3}_{5}$ $G^{\star 3}_{6}$ $G^{\star 3}_{7}$

Figure: A binary partition tree of the dual graph $G^{\star}$

3. The graph wavelet packet vectors in $G^{\star j}_{k}$ can be generated as follows:

$$\boldsymbol{\psi}^{j}_{k,l} = \Phi F^{j}_{k} \Phi^{\mathsf{T}} \boldsymbol{e}_{l} \quad \text{for } j = 0 : j_{\max},\ k = 0 : 2^{j} - 1,\ l = 0 : n - 1$$

in which, the diagonal matrix $F^{j}_{k} \in \mathbb{R}^{n \times n}$ with $F^{j}_{k}[l, l] = \chi_{V^{\star j}_{k}}(l)$, $l = 0 : n - 1$, which selects the eigenvectors corresponding $V^{\star j}_{k}$, Φ is the eigenvector matrix, and $\boldsymbol{e}_{l}$ is the canonical basis vector at the lth vertex.

An Ideal Case: Shannon Wavelets from DCT

- We can generate *Shannon wavelets* from the graph Laplacian eigenvectors of a 1D path (i.e., the DCT-II basis vectors) by simply setting $F_0^j = \mathrm{diag}(\mathbf{1}_{n/2^j}, \mathbf{0}_{n-n/2^j})$; $F_1^j = \mathrm{diag}(\mathbf{0}_{n/2^j}, \mathbf{1}_{n/2^j}, \mathbf{0}_{n-n/2^{j-1}})$, and computing $\boldsymbol{\phi}_l^j = \Phi F_0^j \Phi^\top \boldsymbol{e}_l$ (father); $\boldsymbol{\psi}_l^j = \Phi F_1^j \Phi^\top \boldsymbol{e}_l$ (mother).

- Can generate smoother wavelets (e.g., Meyer wavelets) by using *smoother partition of unity* in the diagonals of F_*^j's

An Ideal Case: Shannon Wavelets from DCT

- We can generate *Shannon wavelets* from the graph Laplacian eigenvectors of a 1D path (i.e., the DCT-II basis vectors) by simply setting $F_0^j = \mathrm{diag}(\mathbf{1}_{n/2^j}, \mathbf{0}_{n-n/2^j})$; $F_1^j = \mathrm{diag}(\mathbf{0}_{n/2^j}, \mathbf{1}_{n/2^j}, \mathbf{0}_{n-n/2^{j-1}})$, and computing $\boldsymbol{\phi}_l^j = \Phi F_0^j \Phi^\mathsf{T} \boldsymbol{e}_l$ (father); $\boldsymbol{\psi}_l^j = \Phi F_1^j \Phi^\mathsf{T} \boldsymbol{e}_l$ (mother).

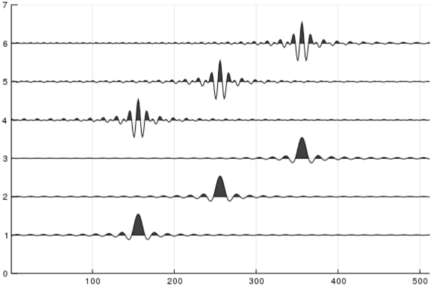


Figure: From DCT to Shannon wavelets ($j = 3$)

- Can generate smoother wavelets (e.g., Meyer wavelets) by using *smoother partition of unity* in the diagonals of F_*^j's

An Ideal Case: Shannon Wavelets from DCT

- We can generate *Shannon wavelets* from the graph Laplacian eigenvectors of a 1D path (i.e., the DCT-II basis vectors) by simply setting $F_0^j = \mathrm{diag}(\mathbf{1}_{n/2^j}, \mathbf{0}_{n-n/2^j})$; $F_1^j = \mathrm{diag}(\mathbf{0}_{n/2^j}, \mathbf{1}_{n/2^j}, \mathbf{0}_{n-n/2^{j-1}})$, and computing $\boldsymbol{\phi}_l^j = \Phi F_0^j \Phi^{\mathsf{T}} \boldsymbol{e}_l$ (father); $\boldsymbol{\psi}_l^j = \Phi F_1^j \Phi^{\mathsf{T}} \boldsymbol{e}_l$ (mother).

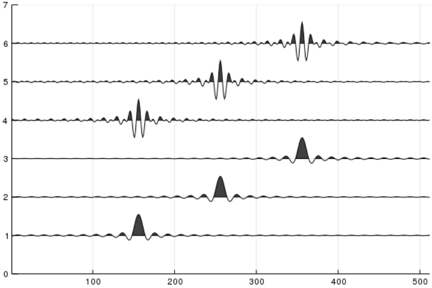
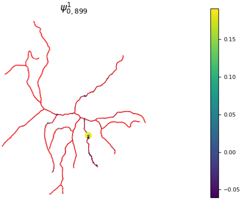


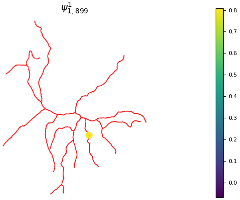
Figure: From DCT to Shannon wavelets ($j = 3$)

- Can generate smoother wavelets (e.g., Meyer wavelets) by using *smoother partition of unity* in the diagonals of F_*^j's

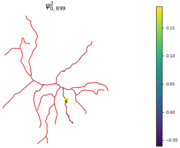
Some wavelet packet vectors on the RGC dendritic tree



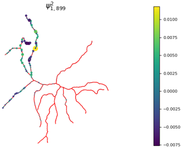
(a) $\psi^1_{0,899}$



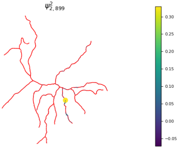
(b) $\psi^1_{1,899}$



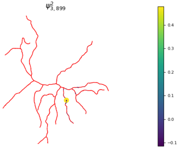
(c) $\psi^2_{0,899}$



(d) $\psi^2_{1,899}$



(e) $\psi^2_{2,899}$



(f) $\psi^2_{3,899}$

Natural Graph Wavelet Basis

- Obviously, the above natural graph wavelet packet dictionary are hugely redundant, containing approximately $n(2n-1)$ basis vectors.
- Constructing a standard wavelet packet dictionary with $n(1+\log_2 n)$ basis vectors, we only need a subset of $\{\boldsymbol{e}_l\}_{l=0:n-1}$ so that the number of basis vectors to generate on $G^{\star j}_k$ is $|V^{\star j}_k|$ (if $n = 2^{j_{\max}}$ with the perfectly balanced binary tree, $|V^{\star j}_k| = 2^{j_{\max}-j}$ where $j_{\max} = \log_2 n$).
- One possibility is to deploy *QR factorization with column pivoting* on $\Phi F^j_k \Phi^{\mathsf{T}}$ by setting its rank to be $|V^{\star j}_k|$.
- Once this is done, one can apply the *best-basis selection algorithm* of Coifman-Wickerhauser or its variants by the Saito group to choose the most suitable basis for a given task (e.g., efficient approximation, denoising, classification, regression, etc.). Note that the best-basis algorithm searches the best one among more than $(1.5)^n$ possible ONBs from the wavelet packet dictionary.

Outline

1. Motivations
2. Measuring Differences between Eigenvectors
3. Numerical Experiments
4. Organizing Laplacian Eigenvectors of Dendritic Trees
5. Other Methods for Eigenvector Organization
6. Building Natural Graph Wavelets
7. Summary

Summary and Future Projects

- Found a *natural* method to order graph Laplacian eigenvectors $\{\boldsymbol{\phi}_i\}_{i=0:n-1}$ using the transportation cost as their mutual distances based on the ROT theory on a fixed graph
- How to examine all possible solutions of Eqn. (*) and find the true cost minimizing transportation plan?
- How to find the *sparsest* nonnegative solution of Eqn. (*) ?
- How to select the best $\alpha \in [0,1]$?
- Which way should we turn $\boldsymbol{\phi}_i$ into $\boldsymbol{p}_i$?
- How to choose a good metric among several possibilities (ROT; TSD; DAG; . . .)?
- How to improve the hierarchical partitioning of the dual graph without forcing recursive binary partitions?
- How to reduce computational complexity for solving Eqn. (*) and for repeated use of QR factorization with column pivoting?

References

- N. Saito & 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, & E. Woei: "Mysteries around graph Laplacian eigenvalue 4," *Linear Algebra Appl.*, vol. 438, no. 8, pp. 3231–3246, 2013.
- J. Irion & N. Saito: "The generalized Haar-Walsh transform," in *Proc. 2014 IEEE Workshop on Statistical Signal Processing*, pp. 472–475, 2014.
- J. Irion & N. Saito: "Applied and computational harmonic analysis on graphs and networks," in *Wavelets and Sparsity XVI, Proc. SPIE 9597*, Paper # 95971F, 2015.
- J. Irion & N. Saito: "Efficient approximation and denoising of graph signals using the multiscale basis dictionaries," *IEEE Trans. Signal and Inform. Process. Netw.*, vol. 3, no. 3, pp. 607–616, 2017.
- 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].
- H. Li & N. Saito: "Metrics of graph Laplacian eigenvectors," in *Wavelets and Sparsity XVIII, Proc. SPIE 11138*, 2019, to appear.
- A. Cloninger, H. Li, and N. Saito: "Natural graph wavelet packets," in preparation, 2019.

Thank you very much for your attention!