#### The First Steps toward Building Natural Graph Wavelets

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Graph Signal Processing Workshop University of Minnesota, Minneapolis, MN June 6, 2019

### Outline

#### Motivations

- 2 Measuring Differences between Eigenvectors
- Output State St
  - Organizing Laplacian Eigenvectors of Dendritic Trees
- 5 Other Methods for Eigenvector Organization
- 6 Further Plan for Building Natural Graph Wavelets

#### Summary

# Acknowledgment

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

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- 2 Measuring Differences between Eigenvectors
- 3 Numerical Experiments
- 4 Organizing Laplacian Eigenvectors of Dendritic Trees
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#### **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 is wrong other than very simple graphs, e.g., undirected unweighted paths and cycles.

### A Simple Yet Important Example: A Path Graph



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  $L_{sym} = D^{-\frac{1}{2}}LD^{-\frac{1}{2}}$  are the *DCT Type I* basis! (See G. Strang, "The discrete cosine transform," *SIAM Review*, vol. 41, pp. 135–147, 1999).

•  $\lambda_k = 2 - 2\cos(\pi k/n) = 4\sin^2(\pi k/2n), \ k = 0: n-1.$ 

•  $\phi_k(\ell) = a_{k;n} \cos\left(\pi k \left(\ell + \frac{1}{2}\right)/n\right), \ k, \ell = 0: n-1; \ a_{k;n} \text{ is a const. s.t. } \|\phi_k\|_2 = 1.$ 

• In this simple case,  $\lambda$  (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  $\lambda_1$  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<sub>2</sub>? Even for such a simple situation there are two possibilities: If m > 2n, then λ<sub>2</sub> = λ<sub>(2,0)</sub> < λ<sub>(0,1)</sub>. On the other hand, if n < m < 2n, then λ<sub>2</sub> = λ<sub>(0,1)</sub> < λ<sub>(2,0)</sub>.
- 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, ..., K. Yet we have  $\lambda_{K+1} = \lambda_{(0,1)} = 4\sin^2(\pi/2n)$  and  $\lambda_{K+2}$  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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- 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  $\{\lambda_k\}_{k=0,1,\dots}$ , 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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• How can we quantify the difference between the eigenvectors?

- The usual  $\ell^2$ -distance doesn't work since  $\| \boldsymbol{\phi}_i \boldsymbol{\phi}_i \|_{2} = \sqrt{2} \delta_{i \neq j}$ .
- Consider the *optimal transport theory*!
  - Convert each φ<sub>i</sub> to a probability mass function (pmf) p<sub>i</sub> over a graph
     G (e.g., via squaring each component of φ<sub>i</sub>)
  - Compute the cost to transport p<sub>i</sub> to p<sub>j</sub> 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 ∈ ℝ<sup>n×n</sup><sub>50</sub>
  - Embed the eigenvectors into a lower dimensional Euclidean space, say, ℝ<sup>m</sup>, m ≪ 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?

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### Ramified Optimal Transportation (ROT) by Q. Xia

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



• 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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### ROT: Discrete Version

Definitions: Two discrete mass distributions (aka atomic measures) in ℝ<sup>d</sup>: a := ∑<sub>i=1</sub><sup>k</sup> m<sub>i</sub>δ<sub>x<sub>i</sub></sub>; b := ∑<sub>j=1</sub><sup>l</sup> n<sub>j</sub>δ<sub>y<sub>j</sub></sub>; {x<sub>i</sub>}<sub>i</sub>, {y<sub>j</sub>}<sub>j</sub> ⊂ ℝ<sup>d</sup>; ∑<sub>i=1</sub><sup>k</sup> m<sub>i</sub> = ∑<sub>j=1</sub><sup>l</sup> n<sub>j</sub>.
Let Path(a, b) be all possible transport paths from a to b without cycles (Xia could manage to remove cycles), i.e., each G ∈ Path(a, b) is a weighted acyclic directed graph with {x<sub>i</sub>}<sub>i</sub> ∪ {y<sub>j</sub>}<sub>j</sub> ⊂ V(G), whose edge weights (>0) satisfy the Kirchhoff law at each interior node v ∈ V(G) \ {x<sub>i</sub>, y<sub>j</sub>}<sub>i,j</sub>:

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

• Define the cost of a transport path  $G \in Path(a, b)$ :

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

# ROT: Discrete Version ...

Xia further derived:

- Number of branching nodes in Path(*a*, *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 Path(a, b).
- The minimum transportation cost d<sub>α</sub>(**a**, **b**) := min<sub>G∈Path(**a**, **b**)</sub> M<sub>α</sub>(G) is a metric on the space of atomic measures of equal mass and is of homogeneous of degree α, i.e., d<sub>α</sub>(λ**a**, λ**b**) = λ<sup>α</sup>d<sub>α</sub>(**a**, **b**), ∀λ > 0.
- Numerical algorithms to compute the α-optimal path for a given pair (a, b).

#### **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  $\tilde{G}$ .
- 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  $\boldsymbol{q}_k[l] = 0$ .

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

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

#### Our Method to Compute Transportation Costs ....

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

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

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

#### Our Method to Compute Transportation Costs ....

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

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

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  $D = (D_{ij})$ :

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

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

1

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#### 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 (\*)

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 $\mathbb{R}^2$ ; $\alpha = 1$



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

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



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

- Generating  $\phi_i^2$  is not the only way to turn  $\phi_i$  into a pmf  $p_i$ .
- Other examples include:
  - Normalized  $\ell^1$ :  $\phi_i^1 := (|\phi_i[0]|, ..., |\phi_i[n-1]|)^T / ||\phi_i||_1;$
  - 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:  $\phi_i^e := \exp(\phi_i) / \|\exp(\phi_i)\|_1.$ 

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



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



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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;
- 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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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;  $\lambda_{1141} = 3.9994$ 

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

- We know why such localization/phase transition occurs ⇒ 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.
- Any physiological consequence? Importance of branching vertices?
- Many such eigenvector localization phenomena have been reported: Anderson localization, scars in quantum chaos, ...
- See also an interesting related work for more general setting and for application in numerical linear algebra: I. Krishtal, T. Strohmer, & T. Wertz: "Localization of matrix factorizations," *Foundations of Comp. Math.*, vol. 15, no. 4, pp. 931–951, 2015.
- 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

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### 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!)

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#### **7** Summary

#### Natural Graph Wavelet Frame

• Given a graph  $G = \{V, E, W\}$  with |V| = n and the distance matrix D of its eigenvectors, we can get a partition of all the eigenvectors based on some clustering method,  $\mathscr{P} = \{\mathscr{C}_1, \mathscr{C}_2, \cdots, \mathscr{C}_N\}, 1 \le N \le n$ , in which

$$\bigcup_{j=1}^N \mathscr{C}_j = \{1, 2, \cdots, n\} \quad \text{and} \quad \mathscr{C}_i \cap \mathscr{C}_j = \emptyset, i \neq j.$$

• In the following notation, the subindex *j* stands for the cluster and the subindex *k* represents the localization.

$$\boldsymbol{\psi}_{k,j} = \Phi \overbrace{F_j \Phi^{\top} \boldsymbol{e}_k}^{\text{Filtering}}$$
 for  $j = 1, 2, \dots, N$  and  $k = 1, 2, \dots, n$ 

in which, the diagonal matrix  $F_j \in \mathbb{R}^{n \times n}$  satisfies  $F_j(l, l) = \chi_{\mathscr{C}_j}(l)$  for  $l = 1, 2, \dots, n, \Phi$  stores all the graph Laplacian eigenvectors, and  $\boldsymbol{e}_k$  is the canonical basis vector at vertex  $v_k$ .

We can show that {Ψ<sub>k,j</sub>}<sub>k=1,...,n;j=1,...,N</sub> is a N times redundant wavelet frame.

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- One way is to *pick n vectors out of nN vectors* in the frame  $\{\psi_{k,j}\}$  by using  $\{e_k\}_{k \in T_j}$ , in which  $T_j \subset \{1, 2, \dots, n\}$ , instead of all  $\{e_k\}_{k=1,\dots,n}$  for each  $\mathscr{C}_j$ , so that  $\sum_{j=1}^N |T_j| = n$ . These *n* vectors may not be mutually orthogonal, so we may need some *orthogonalization procedure*.
- Another way is by *sparsifying rotation*. First, we permute Φ into Φ̂ based on 𝒫: Φ̂ = [φ<sub>𝔅1</sub>, φ<sub>𝔅2</sub>, ..., φ<sub>𝔅N</sub>] in which 𝔅<sub>j</sub> = {j<sub>1</sub>, j<sub>2</sub>, ..., j<sub>l</sub>} and φ<sub>𝔅j</sub> = [φ<sub>j1</sub>, φ<sub>j2</sub>, ..., φ<sub>jl</sub>]. Then, we rotate Φ̂ within each cluster 𝔅<sub>j</sub> for j = 1, 2, ..., N to get an sparse orthonormal wavelet basis Ψ ∈ ℝ<sup>n×n</sup>.
- Yet another way is *not* to use the MDS embedding and clustering, but use *weighted linear combinations of the eigenvectors* where the weights reflect the *similarity* between them, which can be derived from the *distance matrix* already computed.
- Or ..

- One way is to *pick n vectors out of nN vectors* in the frame {Ψ<sub>k,j</sub>} by using {e<sub>k</sub>}<sub>k∈T<sub>j</sub></sub>, in which T<sub>j</sub> ⊂ {1,2,...,n}, instead of all {e<sub>k</sub>}<sub>k=1,...,n</sub> for each C<sub>j</sub>, so that ∑<sup>N</sup><sub>j=1</sub> |T<sub>j</sub>| = n. These n vectors may not be mutually orthogonal, so we may need some orthogonalization procedure.
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- Find k-nearest neighbor vectors of  $\phi_0$  w.r.t. the ROT distance, which form a space  $V_0$  like in the *multiresolution analysis*
- For each eigenvector in V<sub>0</sub>, find its k-NN vectors, collect them all to form V<sub>1</sub> ⊃ V<sub>0</sub>, which is a space spanned by *father* wavelets
- Then set  $W_0 := V_1 \setminus V_0$ , which is a space spanned by *mother* wavelets

• Iterate this process to have  $V_{j+1} = V_j \oplus W_j$ 

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### 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  $F_0^j = \text{diag}(\mathbf{1}_{n/2^j}, \mathbf{0}_{n-n/2^j})$ ;  $F_1^j = \text{diag}(\mathbf{0}_{n/2^j}, \mathbf{1}_{n/2^j}, \mathbf{0}_{n-n/2^{j-1}})$ , and computing  $\boldsymbol{\psi}_k^j = \Phi F_0^j \Phi^{\mathsf{T}} \boldsymbol{e}_k$  (father);  $\boldsymbol{\psi}_k^j = \Phi F_1^j \Phi^{\mathsf{T}} \boldsymbol{e}_k$  (mother).

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

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The 1st Steps

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#### 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 Further Plan for Building Natural Graph Wavelets

#### 7 Summary

#### Summary and Future Projects

- Found a *natural* method to order graph Laplacian eigenvectors
   {φ<sub>i</sub>}<sub>i=0:n-1</sub> 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  $\phi_i$  into  $p_i$ ?
- How to improve computational complexity for solving Eqn. (\*) ?
- How to choose a good metric among several possibilities (ROT; TSD; DAG; ...)?
- How to proceed to *the Littlewood-Paley theory truly adapted to the graph setting* more precisely like the 1D path case?
- Can apply for comparing more general basis vectors (*not* from eigenvectors) such as those in a wavelet packet dictionary ...

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#### Transportation cost distances in the Haar-Walsh dictionary



#### References

- N. Saito & E. Woei: "Analysis of neuronal dendrite patterns using eigenvalues of graph Laplacians," *Japan SIAM Letters*, vol. 1, pp. 13–16, 2009.
- 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 preparation, 2019.

# Thank you very much for your attention!

Alex Cloninger and I are organizing 3 part minisymposia (12 speakers) on "*Distance Metrics and Mass Transfer Between High Dimensional Point Clouds*" at *ICIAM 2019*, Valencia, Spain on July 17, 2019. So, if you plan to participate in ICIAM 2019, please come to our sessions!

