Natural Constructions of Smooth Graph Wavelet Packets

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in collaboration with
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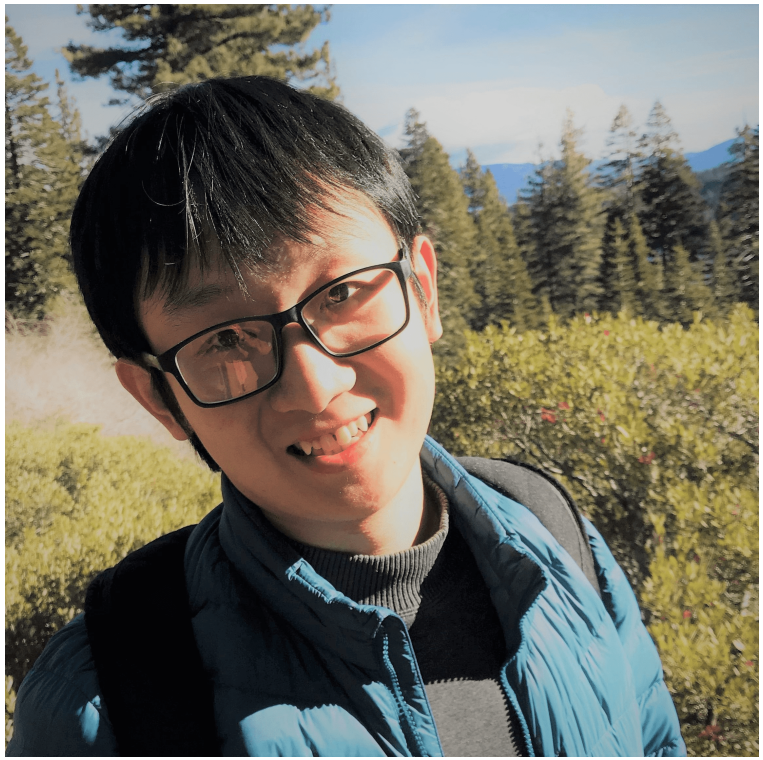
Virtual Workshop on "Time–Frequency Frames and Their Applications"
Research Institute for Mathematical Sciences, Kyoto University, Japan
October 20, 2020

Outline

Acknowledgment

- NSF Grants: DMS-1819222, DMS-1912747, CCF-1934568, DMS-2012266
- ONR Grants: N00014-16-1-2255, N00014-20-1-2381
- Russell Sage Foundation Grant #2196



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- We are interested in generating a ***smooth*** *wavelet packet dictionary* on a given graph, which truly generalizes its classical counter part.
- We have already developed the *Hierarchical Graph Laplacian Eigen Transform* (HGLET) [J. Irion & N. Saito, 2014a]; the *Generalized Haar-Walsh Transform* (GHWT) [J. Irion & N. Saito, 2014b]; and its extension *eGHWT* [Y. Shao & N. Saito, 2019].
- HGLET is a graph version of the *Hierarchical Block Discrete Cosine Transform* (BDCT) while GHWT/eGHWT are graph versions of the *Haar-Walsh wavelet packet transform* [R. Coifman & Y. Meyer, 1989]/the *adapted time-frequency tilings* [C. Thiele & L. Villemoes, 1996].
- All of these methods require the *hierarchical bipartition tree* of an input graph G, and the support of each basis vector is restricted within the partition pattern. That is, for a given pair of mutually exclusive subgraphs of G, the support of the basis vectors of one of such subgraphs does *not smoothly crossover* to the other subgraph.

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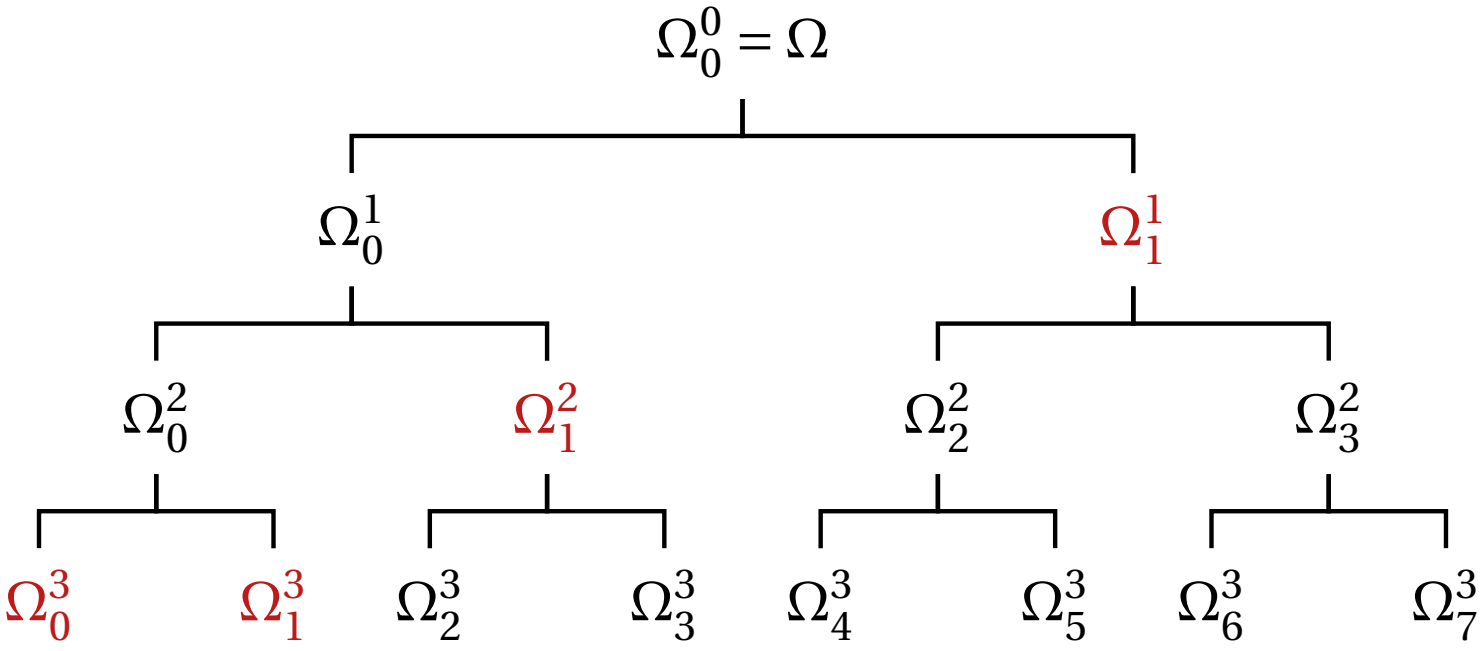

Figure: A binary partition tree of the input space Ω

- 1D Hierarchical BDCT $\Longleftrightarrow \Omega = [0,1]$ on the spatial axis
- HGLET, GHWT, eGHWT $\Longleftrightarrow \Omega = G$, a graph
- Classical wavelet packets $\Longleftrightarrow \Omega = [0, \frac{1}{2}]$ on the *frequency* axis
- *Smooth graph wavelet packets* $\Longleftrightarrow \Omega =$??

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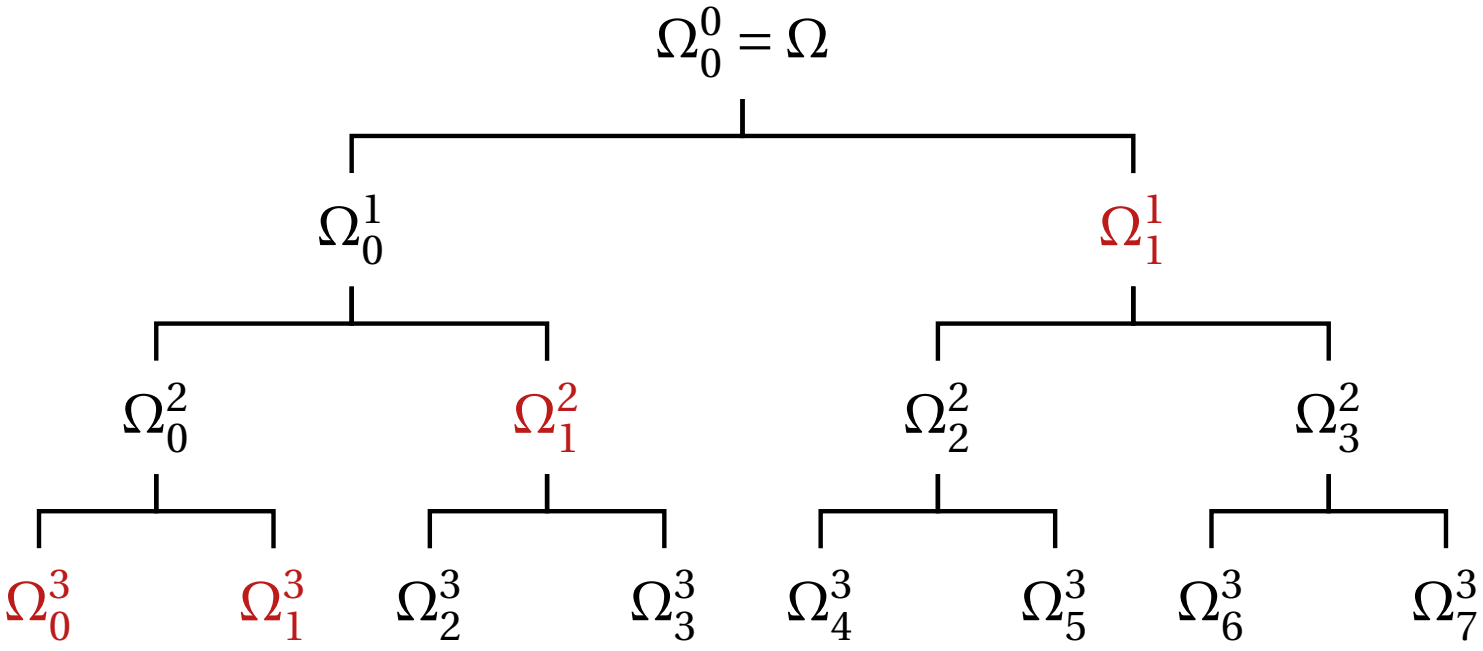

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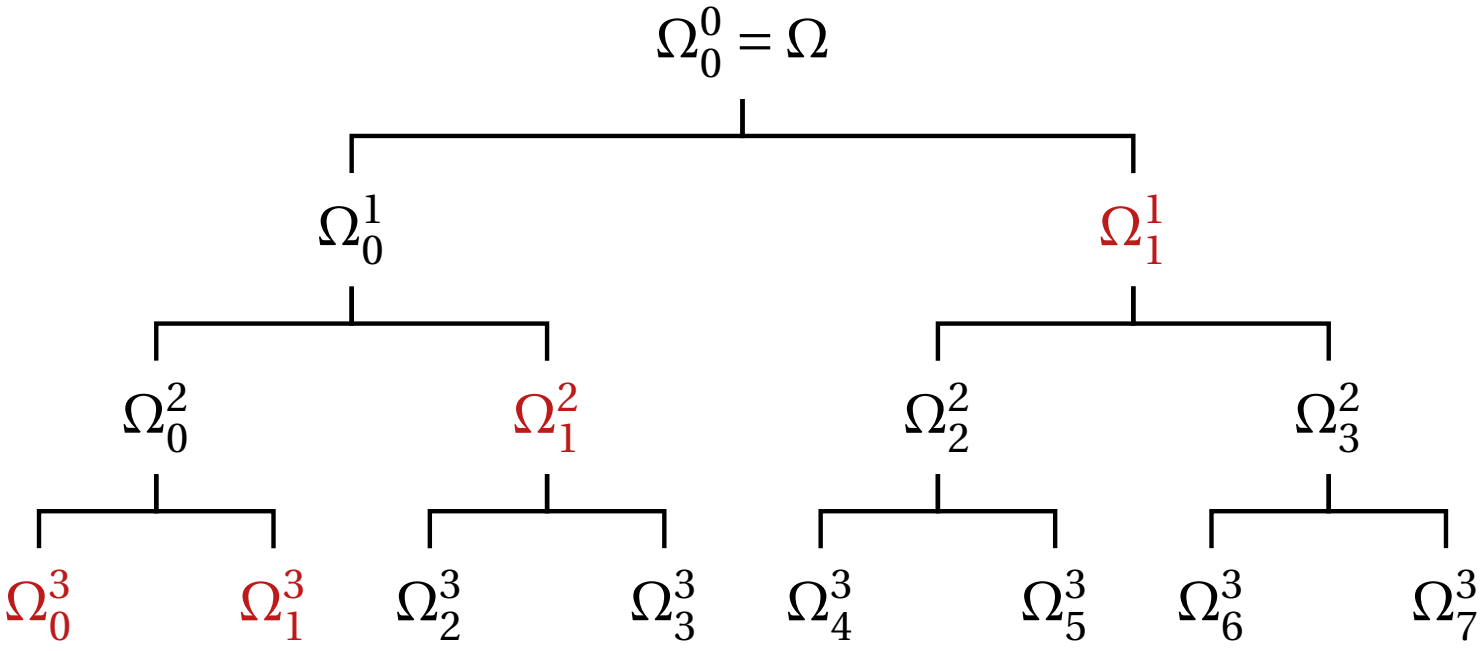

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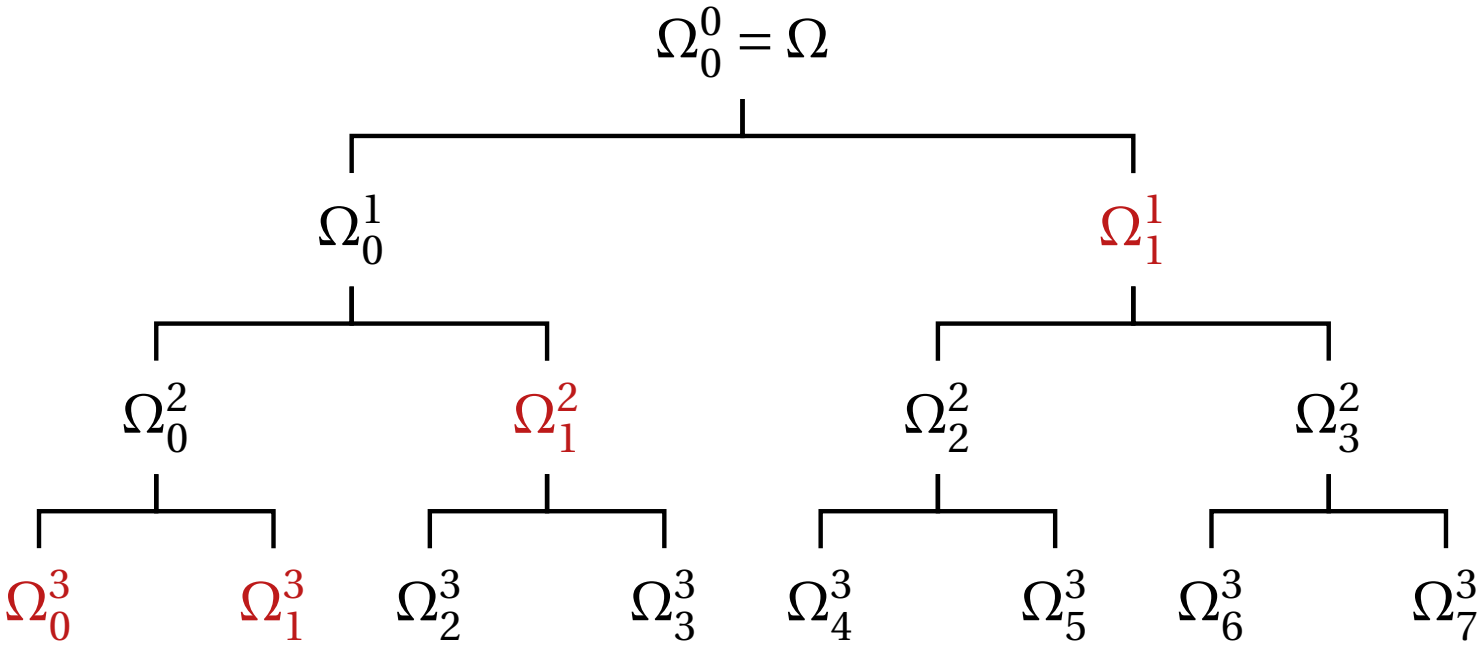

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Problems of Interpreting "eigenvalues ≈ frequencies^2"

- 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; Fourier modes on graphs may be quite different from those on regular lattices.
- 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* $L_{\mathrm{sym}} = D^{-\frac{1}{2}} L D^{-\frac{1}{2}}$ 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.*

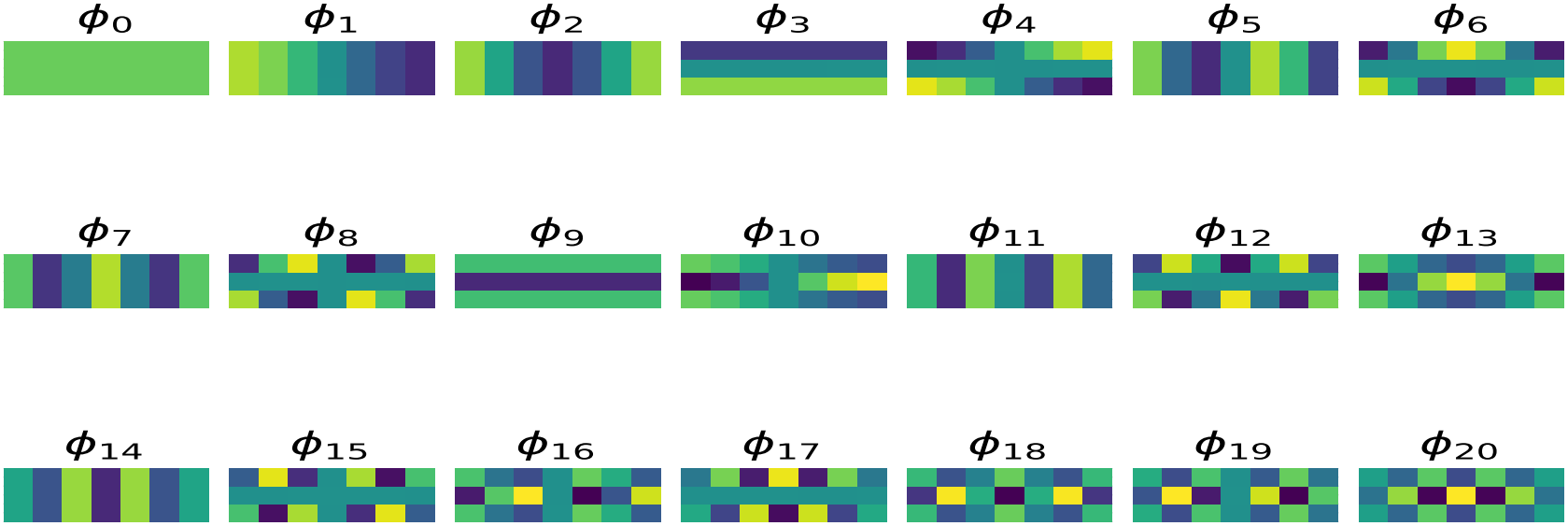
Problem with 2D Lattice Graph

- As soon as the domain becomes *even slightly more complicated than* unweighted and undirected paths/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:

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

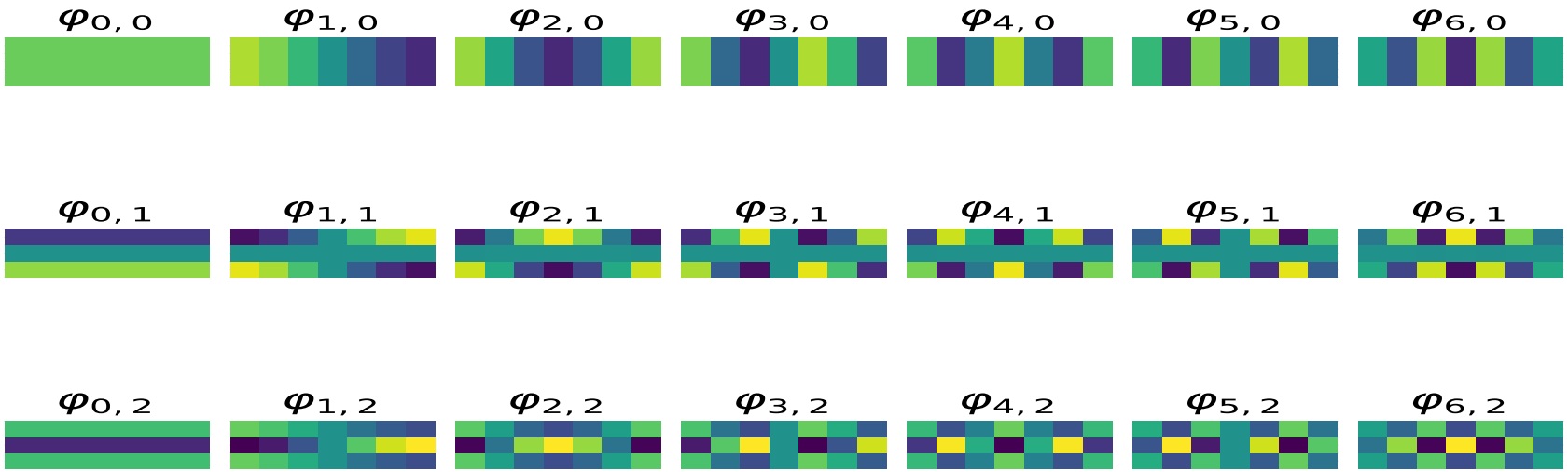
$$\phi_k(x,y) = a_{k_x;m}\, a_{k_y;n} \cos\left(\frac{\pi k_x}{m}\left(x+\frac{1}{2}\right)\right)\cos\left(\frac{\pi k_y}{n}\left(y+\frac{1}{2}\right)\right),$$

  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.

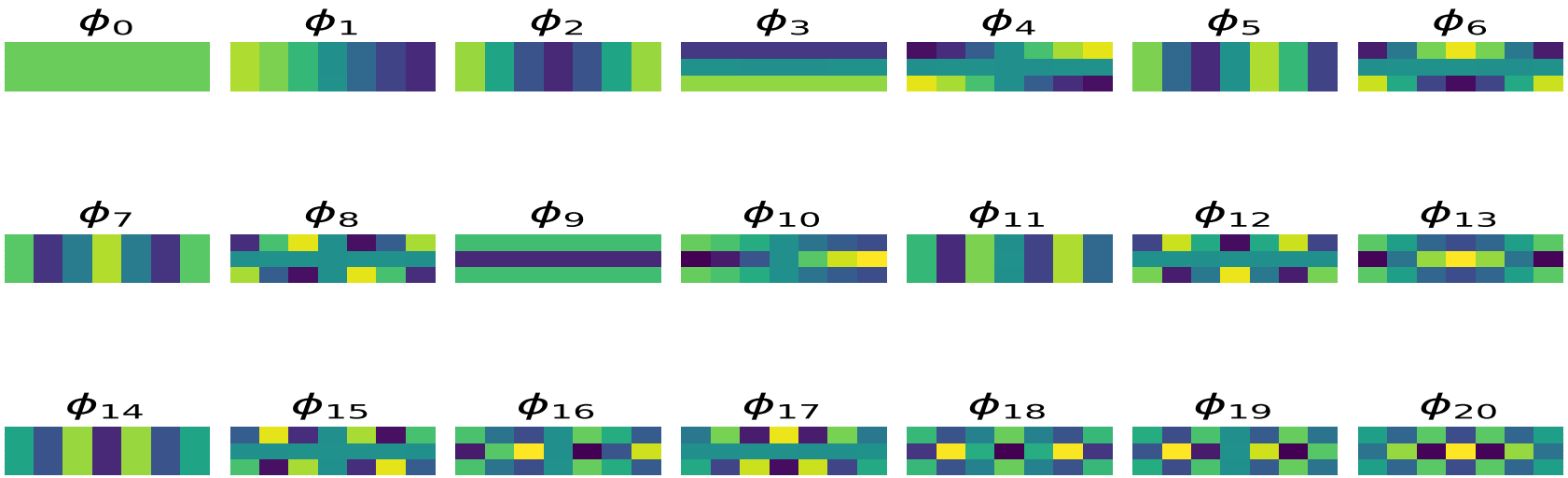


- All of a sudden the eigenvalue of a completely different type of oscillation sneaks into the eigenvalue sequence.
- Hence, on a general domain or a general graph, by simply looking at the Laplacian eigenvalue sequence $\{\lambda_k\}_{k=0,1,\ldots}$, it is *almost impossible to organize the eigenpairs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



instead of



Outline

Plan

- How can we *quantify the difference between the eigenvectors*?
- The usual ℓ^2-distance doesn't work since $\left\|\boldsymbol{\phi}_i - \boldsymbol{\phi}_j\right\|_2 = \sqrt{2}\delta_{i\neq j}$.
- Need to come up with a metric that quantifies the "behavioral" differences between any pair of eigenvectors. Having such a metric, we do the following:

1. Choose a metric and compute the "distance" between $\boldsymbol{\phi}_i$ and $\boldsymbol{\phi}_j$ for all $i, j = 0 : n-1$, which results in a "distance" matrix $D \in \mathbb{R}^{n\times n}_{\geq 0}$
2. Construct a *dual graph* $G^\star(V^\star, E^\star)$ where the ith node corresponds to $\boldsymbol{\phi}_i$, and the weight of the edge (i, j) is the *affinity* between $\boldsymbol{\phi}_i$ and $\boldsymbol{\phi}_j$, e.g., $1/D_{i,j}$ or $\exp(-D^2_{i,j}/\epsilon)$ with some $\epsilon > 0$
3. *Organize* and *group* $V^\star$ to generate *wavelet packet vectors* on G

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Various Metrics for Eigenvector Differences

- A *similarity* measure (HAD) based on the *average of local correlations* of eigenvectors [A. Cloninger & S. Steinerberger, 2018]
- The *ramified optimal transport* (ROT) method [N. Saito, 2018]
- The *difference of absolute gradient* (DAG) method [H. Li & N. Saito, 2019]
- The *time-stepping diffusion* (TSD) method [H. Li & N. Saito, 2019]
- The ROT method seems to work well for transportation networks with hubs (e.g., neuronal dendritic trees) whereas the HAD and DAG methods seem to work well for (ir)regular grids/lattices (e.g., road networks).
- For more pros and cons of these methods, see [H. Li & N. Saito, 2019].

Difference of Absolute Gradient (DAG) Pseudometric

- The basic idea: use the *absolute gradient* of each eigenvector as its feature vector describing its behavior.
- Let $G(V,E)$ be an input graph (connected, undirected, weighted, and simple) with $|V|=n$, $|E|=m$. Let $Q \in \mathbb{R}^{n\times m}$ be its *incidence matrix*. Then, *DAG **pseudo**metric* (*the identity of discernible* is not satisfied) is defined as:

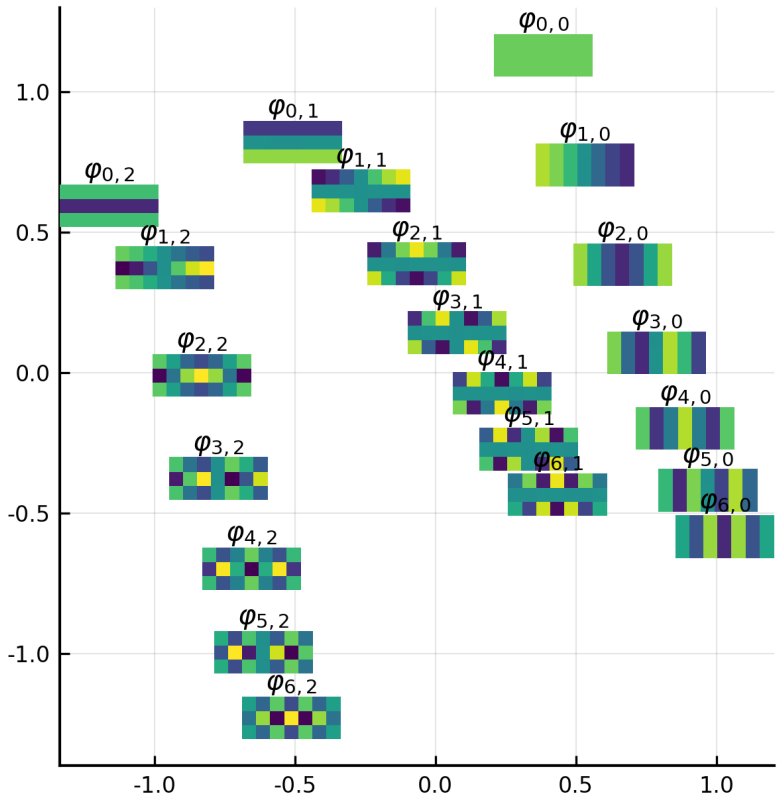
$$d_{\mathrm{DAG}}(\boldsymbol{\phi}_i,\boldsymbol{\phi}_j) := \||\nabla_G|\boldsymbol{\phi}_i - |\nabla_G|\boldsymbol{\phi}_j\|_2 \quad \text{where } |\nabla_G|\boldsymbol{\phi} := \mathrm{abs.}(Q^{\mathsf{T}}\boldsymbol{\phi}) \in \mathbb{R}^m_{\geq 0}$$

- It is related to the *Hadamard product-based affinity* proposed by [A. Cloninger & S. Steinerberger, 2018] as

$$\begin{aligned} d_{\mathrm{DAG}}(\boldsymbol{\phi}_i,\boldsymbol{\phi}_j)^2 &= \left\langle |\nabla_G|\boldsymbol{\phi}_i - |\nabla_G|\boldsymbol{\phi}_j, |\nabla_G|\boldsymbol{\phi}_i - |\nabla_G|\boldsymbol{\phi}_j \right\rangle_E \\ &= \left\langle |\nabla_G|\boldsymbol{\phi}_i, |\nabla_G|\boldsymbol{\phi}_i \right\rangle_E + \left\langle |\nabla_G|\boldsymbol{\phi}_j, |\nabla_G|\boldsymbol{\phi}_j \right\rangle_E - 2\left\langle |\nabla_G|\boldsymbol{\phi}_i, |\nabla_G|\boldsymbol{\phi}_j \right\rangle_E \\ &= \lambda_i + \lambda_j - \sum_{x\in V}\sum_{y\sim x} |\boldsymbol{\phi}_i(x) - \boldsymbol{\phi}_i(y)| \cdot |\boldsymbol{\phi}_j(x) - \boldsymbol{\phi}_j(y)| \quad \text{thanks to } QQ^{\mathsf{T}} = L \end{aligned}$$

  where $\langle\cdot,\cdot\rangle_E$ is the inner product over edges.
- The last term of the formula can be viewed as *a global average of absolute local correlation* between eigenvectors $\Longrightarrow$ the Hadamard-product affinity.
- Given the eigenvectors, *the computational cost is $O(m)$* for each $d_{\mathrm{DAG}}(\cdot,\cdot)$ eval.

2D Lattice $P_7 \times P_3$: d_{DAG} visualized by the classical MDS



- d_{DAG} nicely detects two directions of the oscillations and the eigenvectors are organized naturally in the *2D lattice*.
- For each column of the lattice, the eigenvectors have the same oscillation pattern in the y-direction and the oscillation in the x-direction increases linearly, and vice versa.

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Natural Graph Wavelet Packets: Basic Steps

1. *Bipartition the dual graph $G^\star$ recursively* via any method, e.g., spectral graph bipartition using the *Fiedler vectors*
2. Generate wavelet packet vectors on each subgraph of $G^\star$ that are *well localized on G*

- We refer to the graph wavelet packets generated by the above strategy as *Natural Graph Wavelet Packets* (NGWPs).
- $\exists$ Several possibilities in Step 2; will discuss only one of them today.
- Let $\Phi_0^{(0)} := [\boldsymbol{\phi}_0, \ldots, \boldsymbol{\phi}_{n-1}]$ = a matrix representation of the GL eigenvectors of G = the node set $V^\star$ of $G^\star$, and suppose we get the following *hierarchical bipartition tree* of $\Phi_0^{(0)}$:

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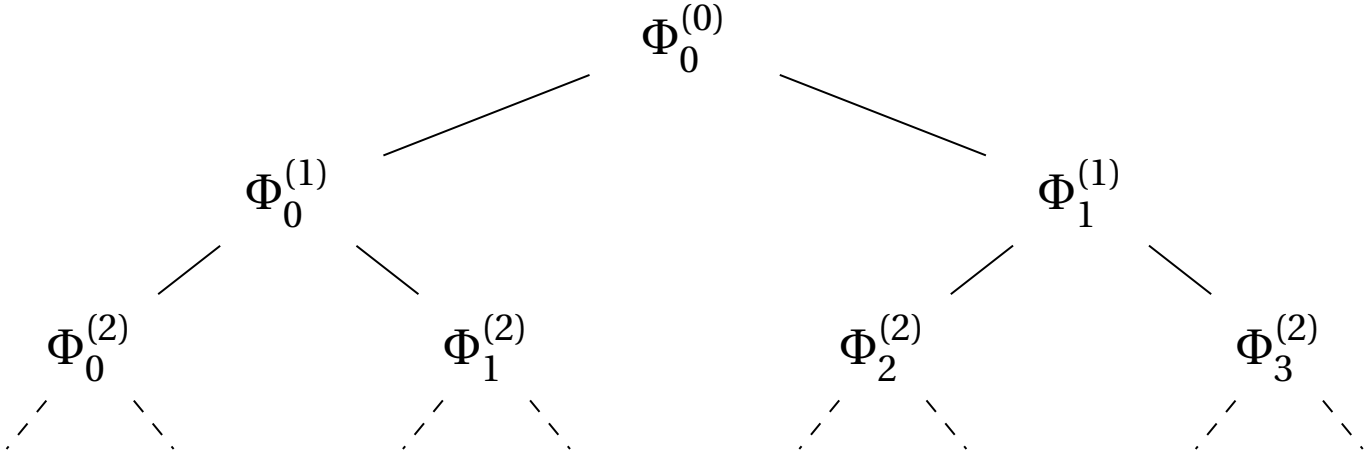


NGWPs by Varimax Rotation

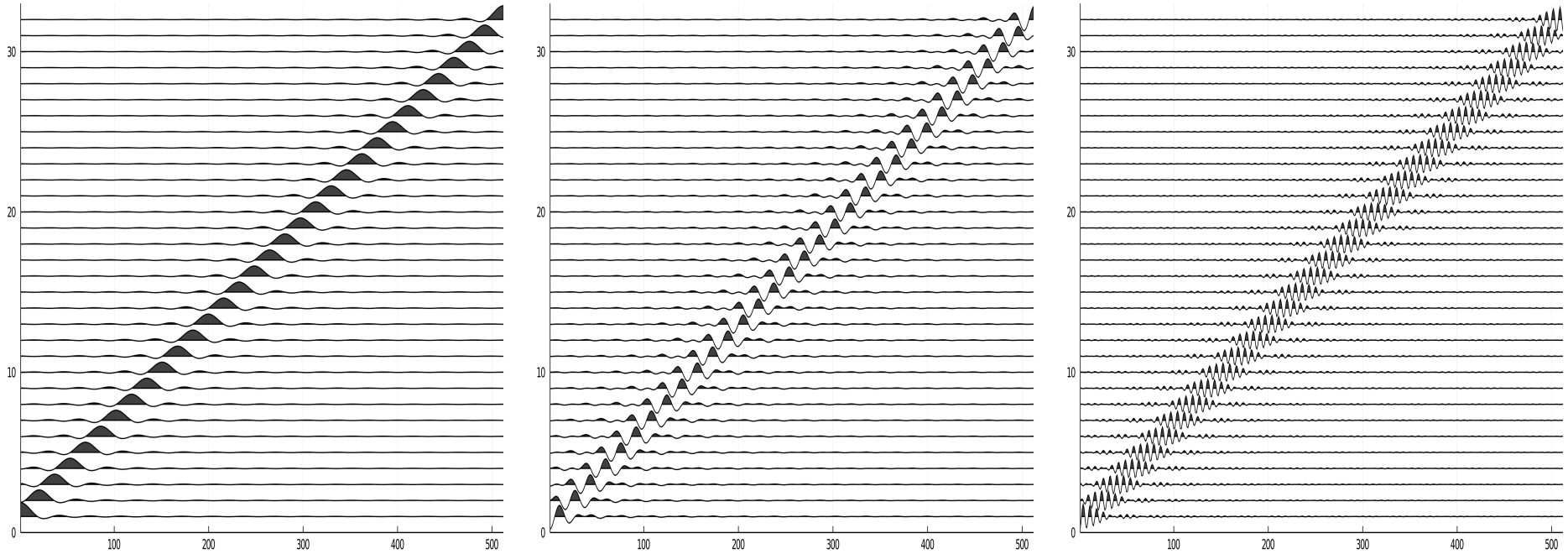
- Given the full binary partition tree of $\Phi_0^{(0)} \in \mathbb{R}^{n\times n}$, perform the *varimax rotation* on $\Phi_k^{(j)} \in \mathbb{R}^{n\times n_k^j}$ for each j and k.
- Varimax rotation [Kaiser (1958); Jennrich (2001)] is an orthogonal rotation, often used in *factor analysis*, to maximize the variances of energy distribution (or a scaled version of the *kurtosis*) of the input column vectors.
- Thanks to the orthonormality of columns of $\Phi_k^{(j)}$, this is equivalent to finding an orthogonal rotation that maximizes the overall *4th order moments*, i.e.,

$$\Psi_k^{(j)} := \Phi_k^{(j)} \cdot R_k^{(j)}, \quad \text{where } R_k^{(j)} = \arg \max_{R\in \mathrm{SO}(n_k^j)} \sum_{p=1}^{n} \sum_{q=1}^{n_k^j} \left[\left(\Phi_k^{(j)} \cdot R \right)^4 \right]_{p,q}.$$

- The column vectors of $\Psi_k^{(j)}$ are *more "localized" in the original domain* G than those of $\Phi_k^{(j)}$. This type of localization is important since the GL eigenvectors in $\Phi_k^{(j)}$ are of *global* nature in general.

The varimax-rotation NGWPs on P_n

are essentially the *Shannon wavelet packets !*



(a) Father wavelet vectors $\Psi_0^{(4)}$

(b) Mother wavelet vectors $\Psi_1^{(4)}$

(c) Wavelet packet vectors $\Psi_4^{(4)}$

Figure: Some of the Shannon wavelet packet vectors on P_{512}

Selecting a Good Natural Graph Wavelet Packet Basis

- Once the NGWP dictionary is built, one can apply the *best-basis selection algorithm* of Coifman-Wickerhauser or its variants developed 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.
- For the examples today, we used the *ℓ^1-norm minimization* to select the best (or *sparsest*) basis among the NGWP dictionary.
- Of course, if one prefers, one can also choose the *wavelet basis* from the NGWP dictionary by selecting the specific subspaces and basis vectors.

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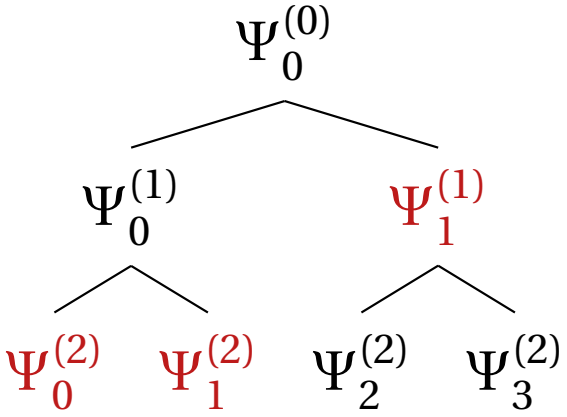
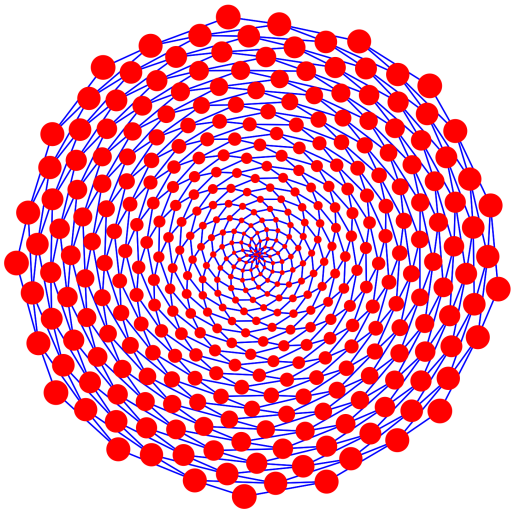
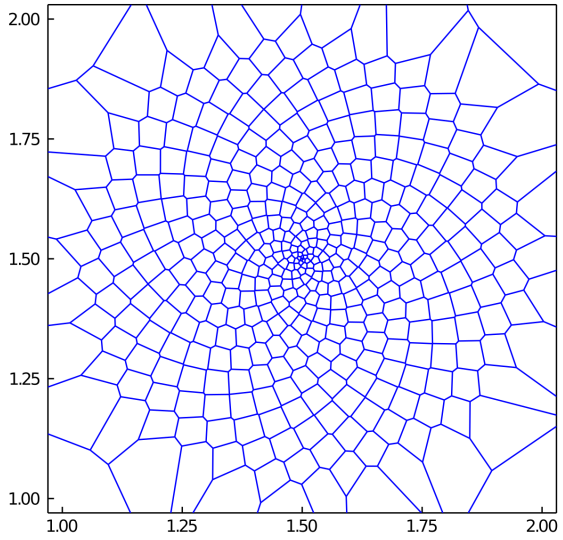


Outline

Example 1: Sunflower Graph



(a) Sunflower graph

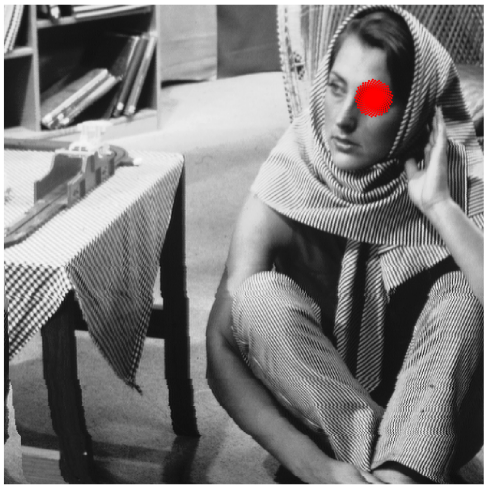


(b) Voronoi tessellation

Figure: (a) Sunflower graph ($n = 400$); (b) Its Voronoi tessellation

- This graph often appears in nature
- Consistent counting of spirals gives rise to *Fibonacci numbers* $0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, \ldots$
- Edge weights = the inverse Euclidean distances between nodes
- My view: a simple model of the distribution of *photoreceptors in mammalian visual systems* due to cell generation and growth

Example 1: Sampling an eye of Barbara by Sunflower Graph



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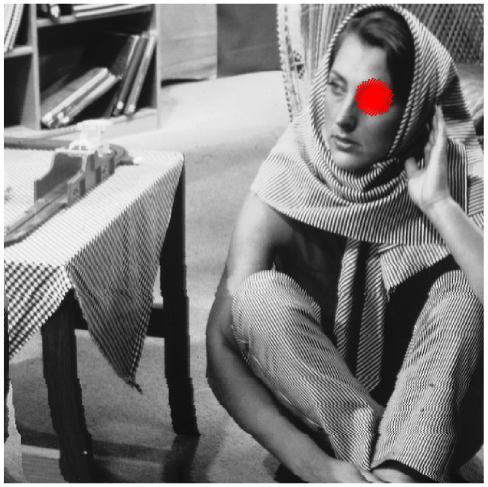

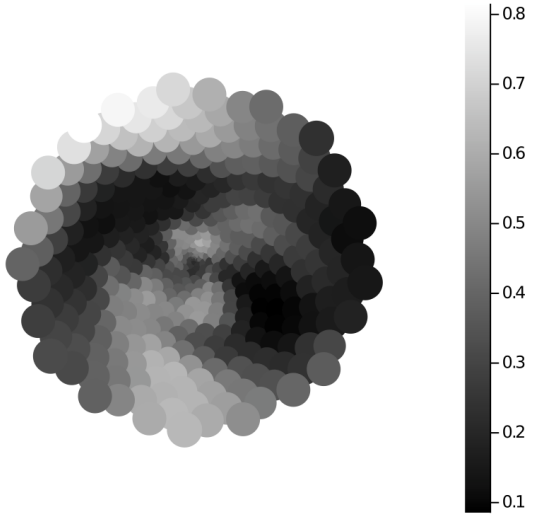

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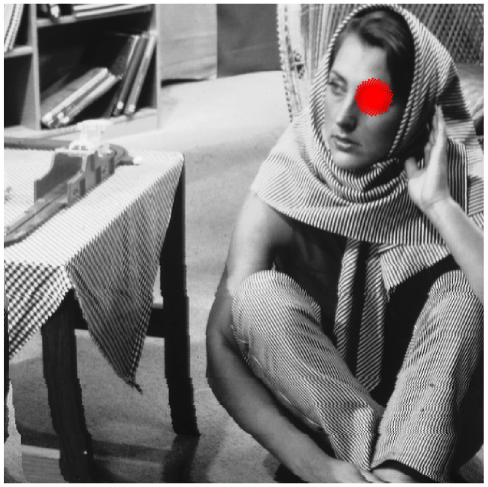
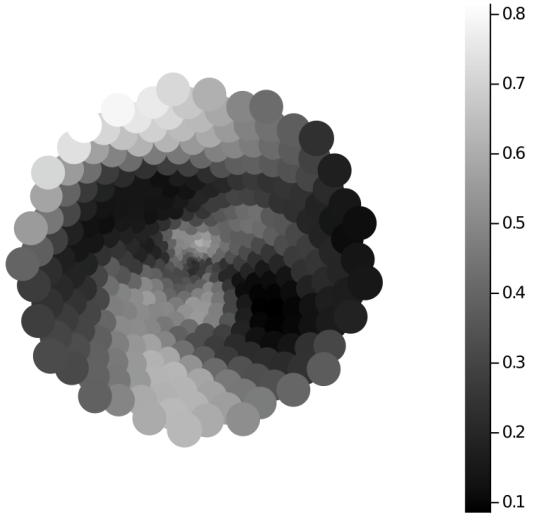
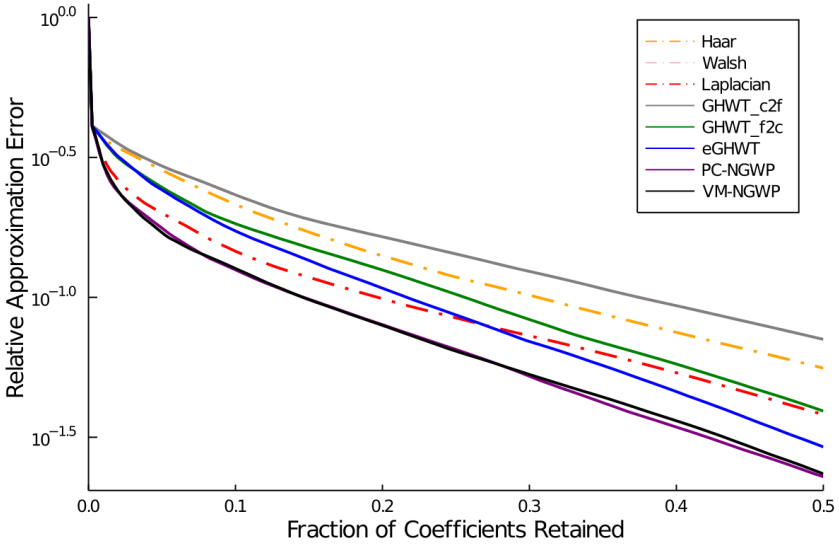
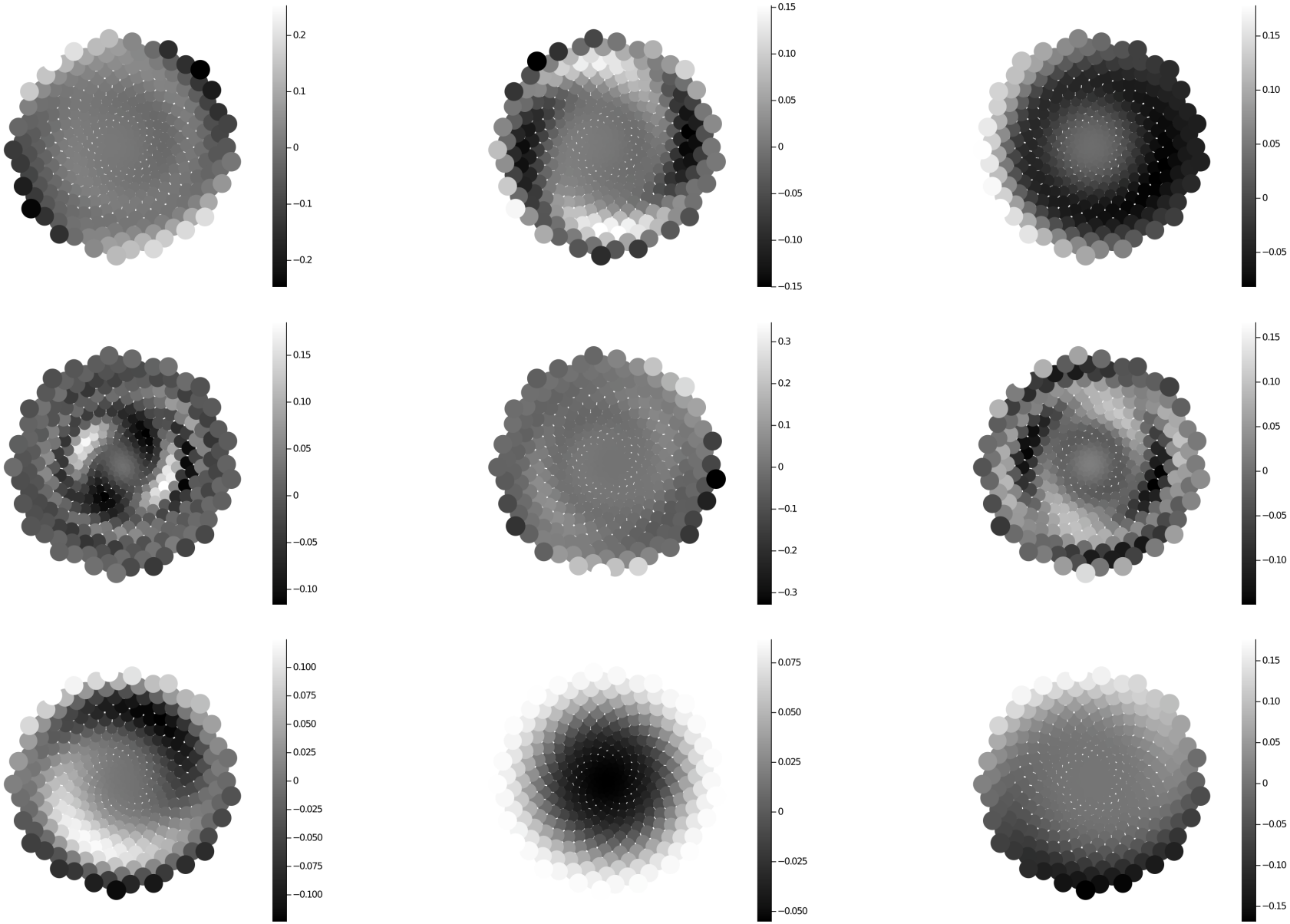






Example 1: Top 9 NGWP vectors for Barbara's eye



Example 1: Sampling cheek of Barbara by Sunflower Graph

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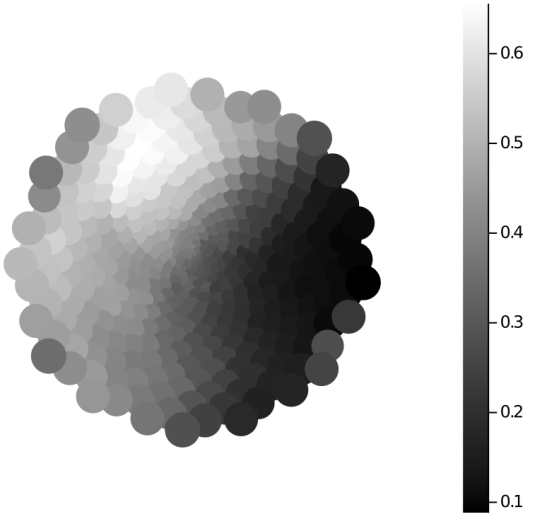

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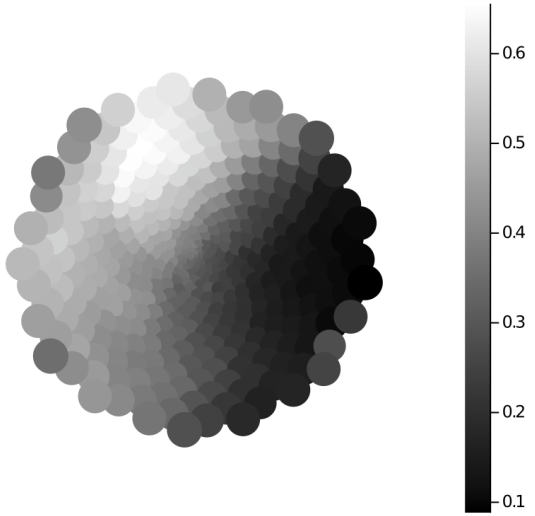

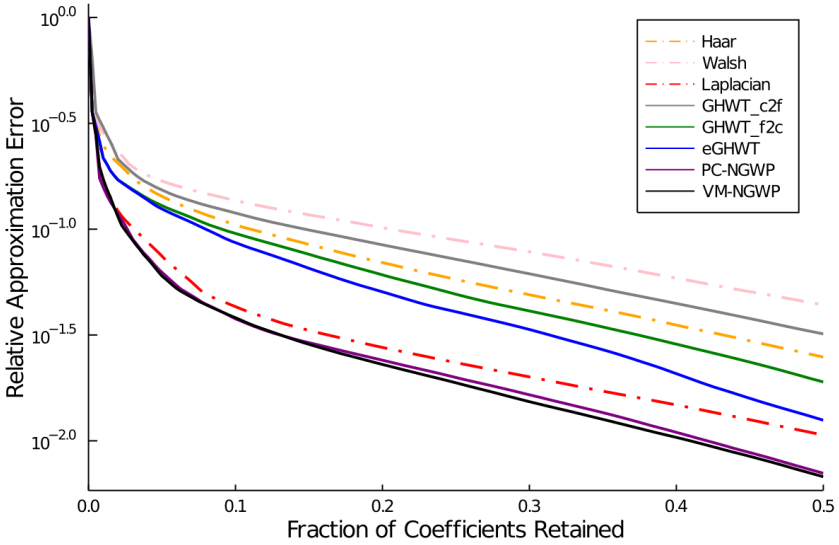

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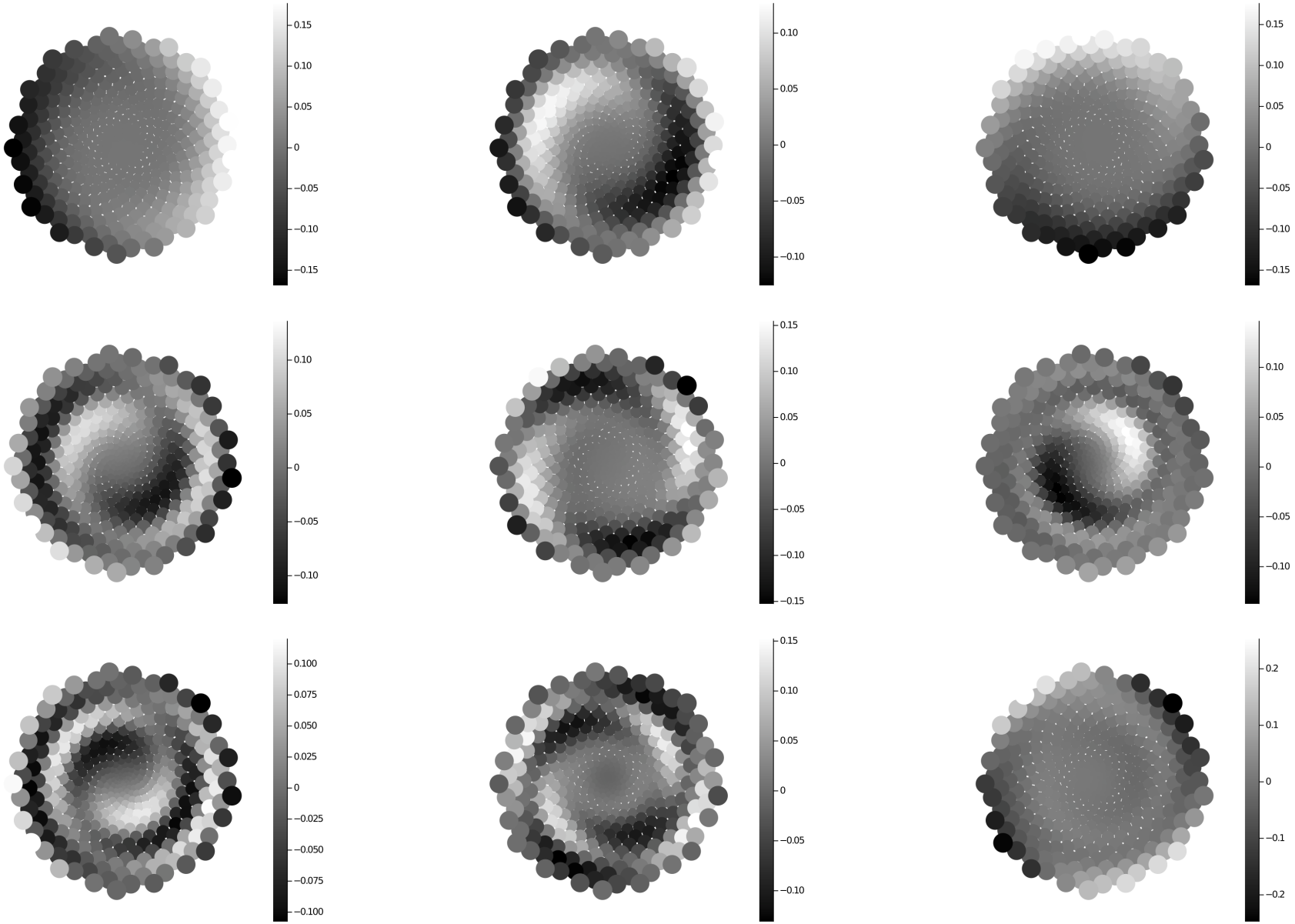
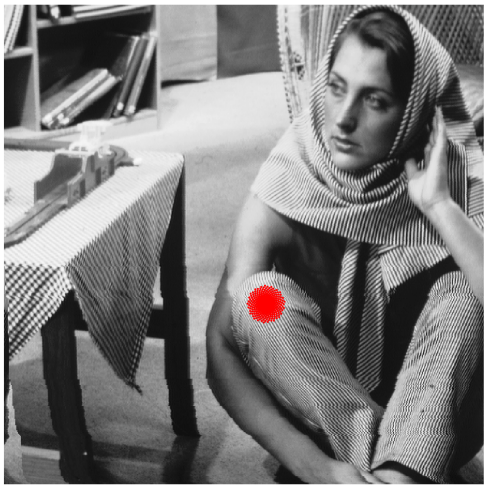


Example 1: Sampling pants of Barbara by Sunflower Graph



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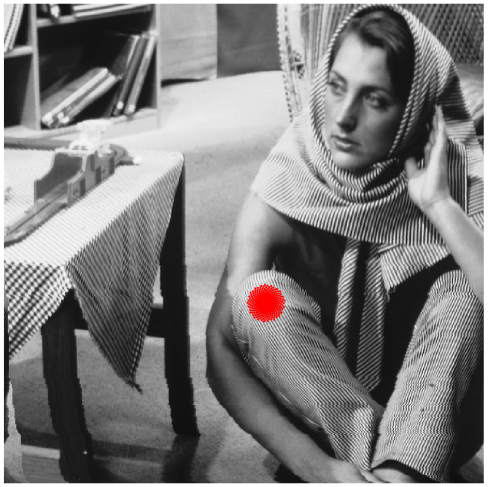

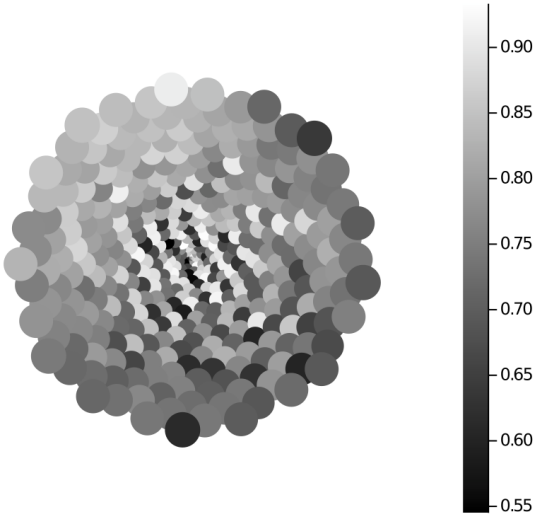

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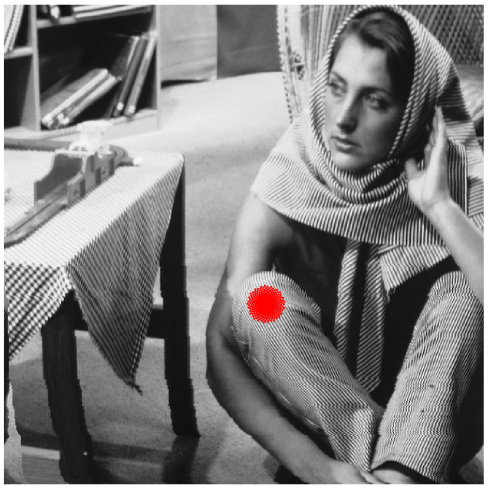

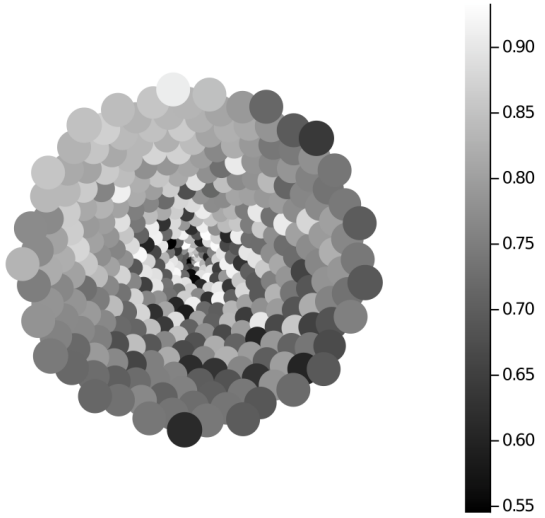

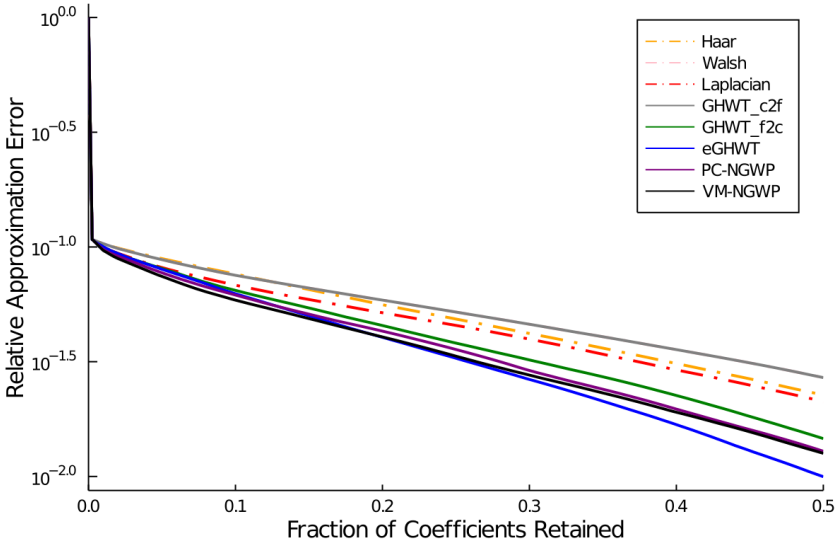

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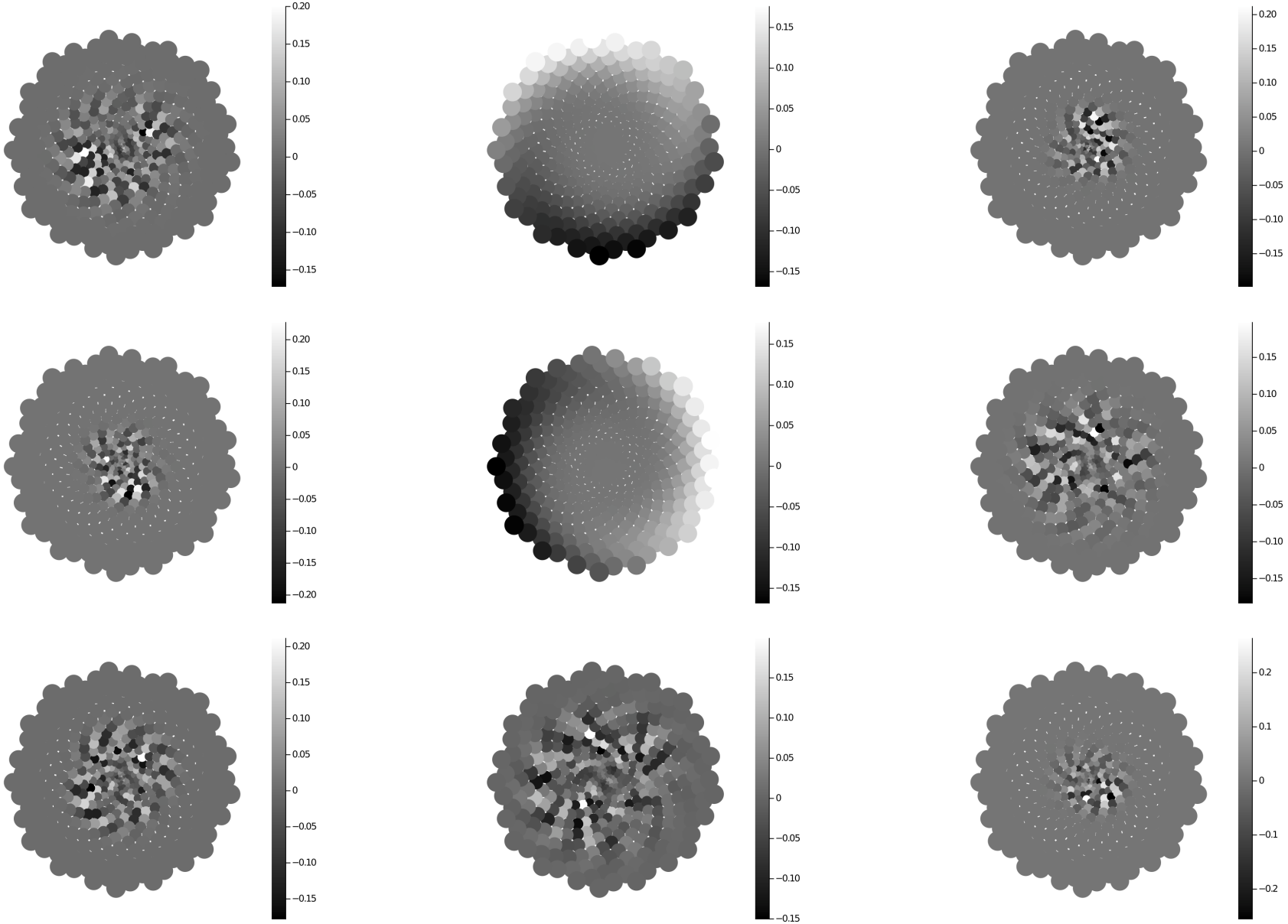


Example 2: Toronto Road Network

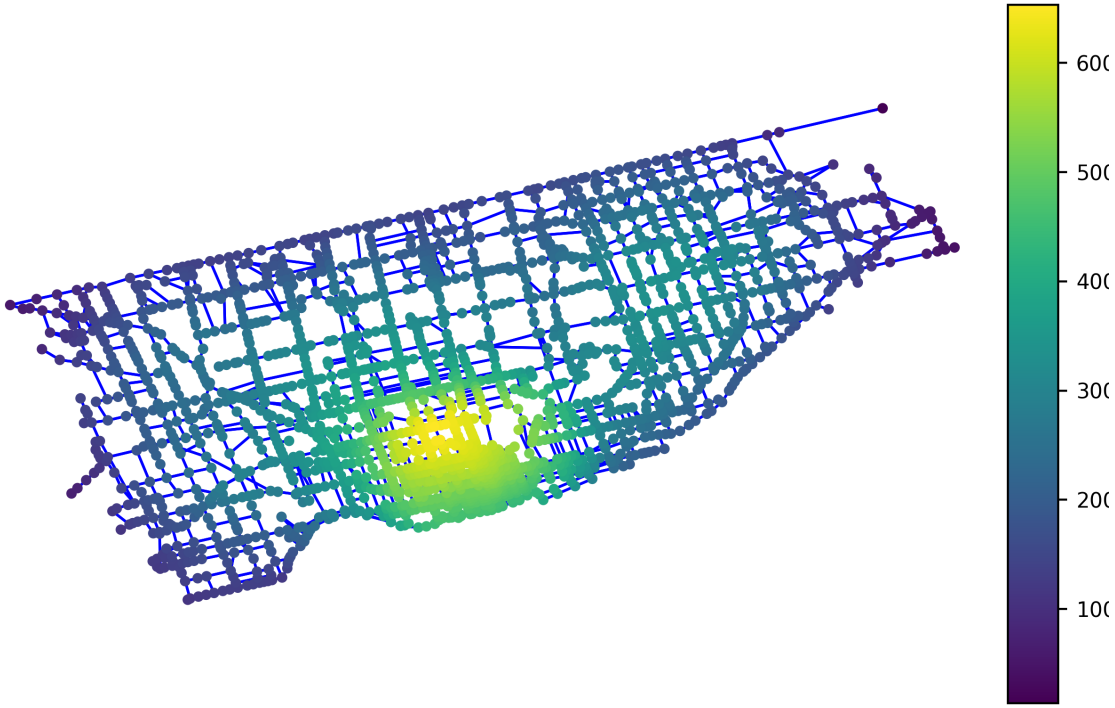
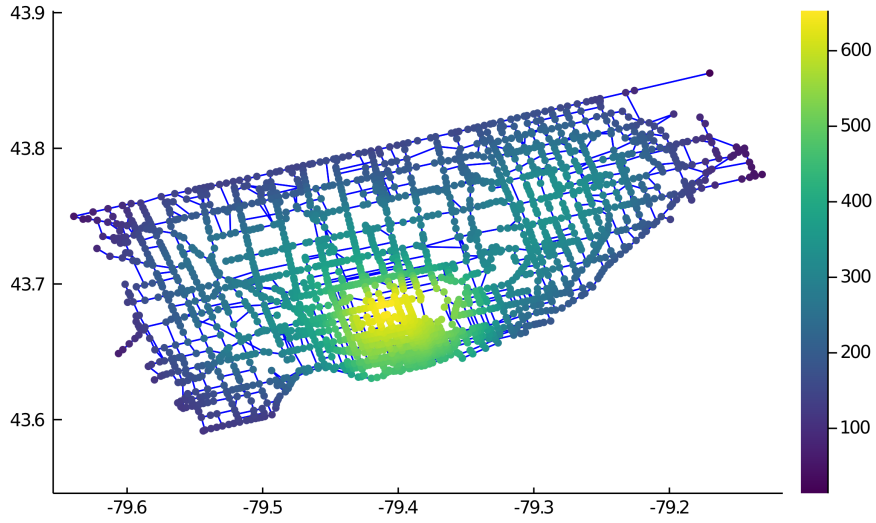


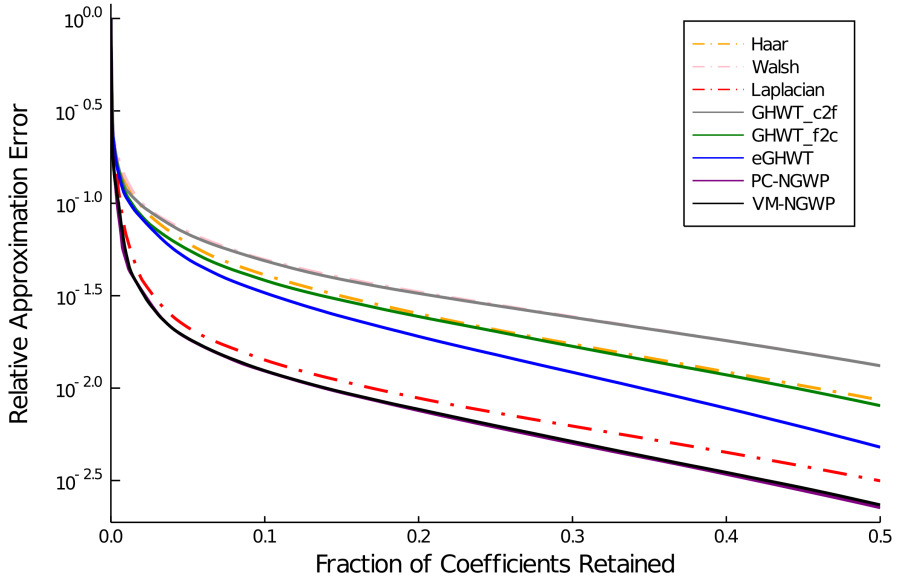
Figure: The road network of Toronto ($n = 2275$ nodes and $m = 3381$ edges)

- Nodes = intersections (with traffic lights); edges = streets
- Edge weights = the inverse Euclidean distances between nodes
- Two graph signals considered: 1) spatial distribution of the street intersections; 2) real pedestrian counts between the hours of 7:30am and 6:00pm on a single day measured during the period 03/22/2004–02/28/2018

Example 2: Smooth Histogram of Street Intersections



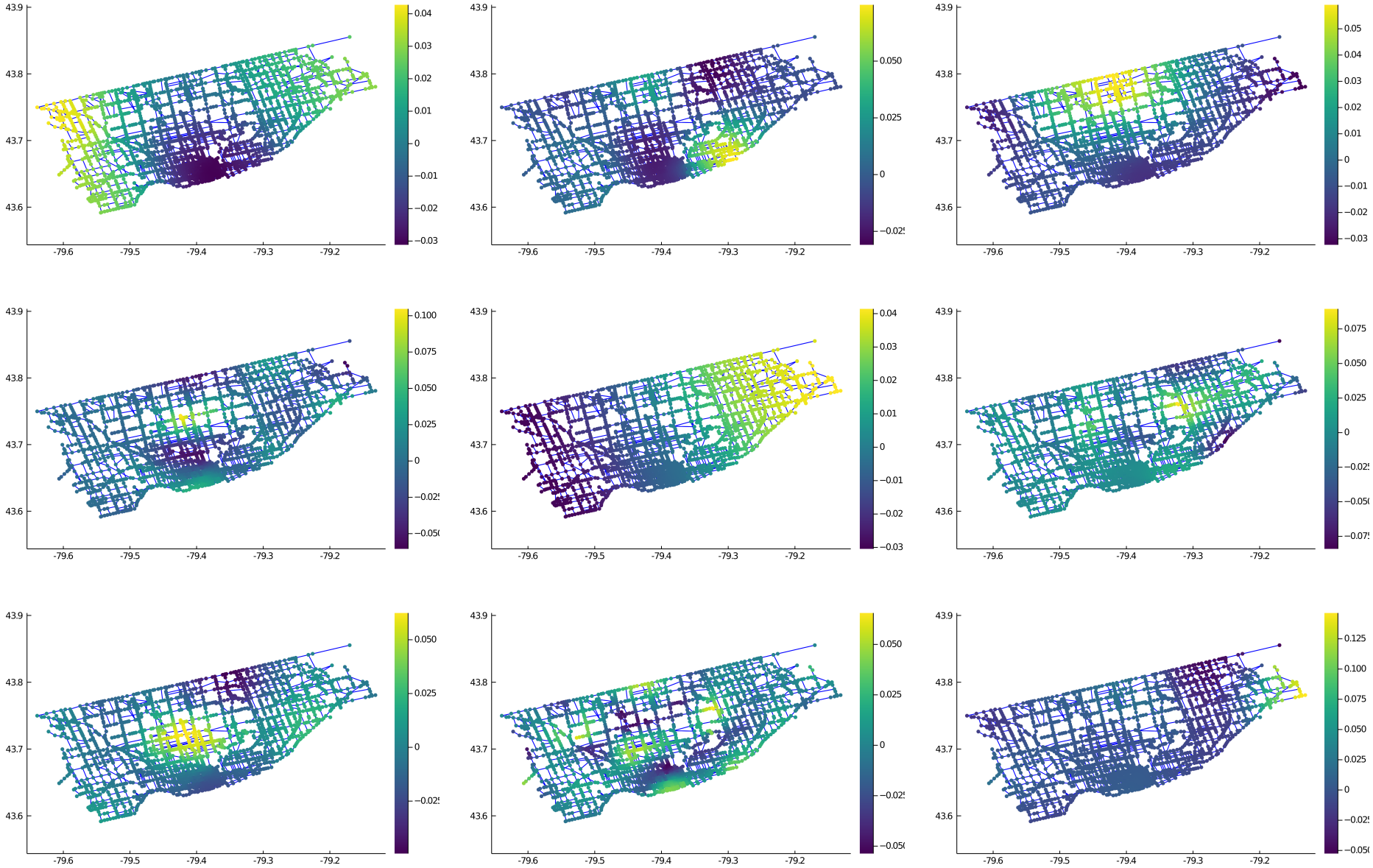
(a) Graph signal



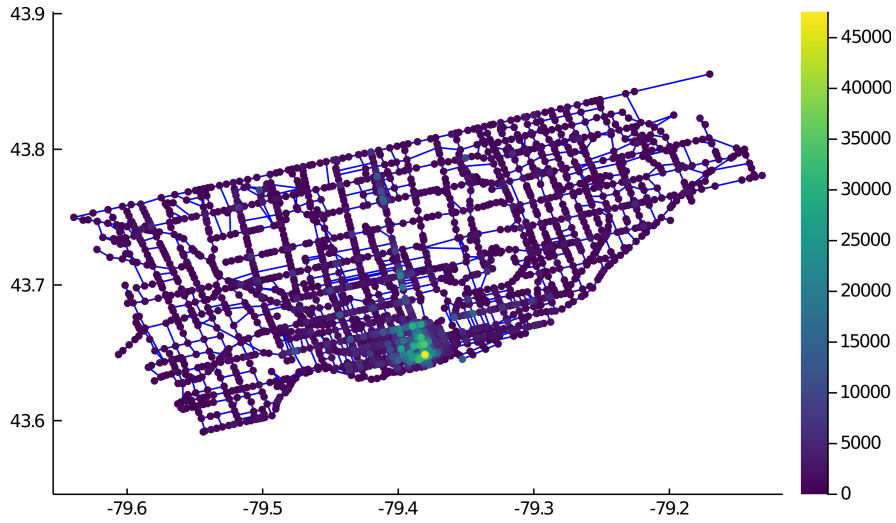
(b) Approximation

Figure: (a) A graph signal representing the smooth spatial distribution of the street intersections on the Toronto street network Toronto; (b) Relative ℓ^2 approximation error of the data shown in (a) vs the fraction of kept coefficients.

Top 9 VM-NGWP best basis vectors



Example 2: Pedestrian Counts at the Intersections



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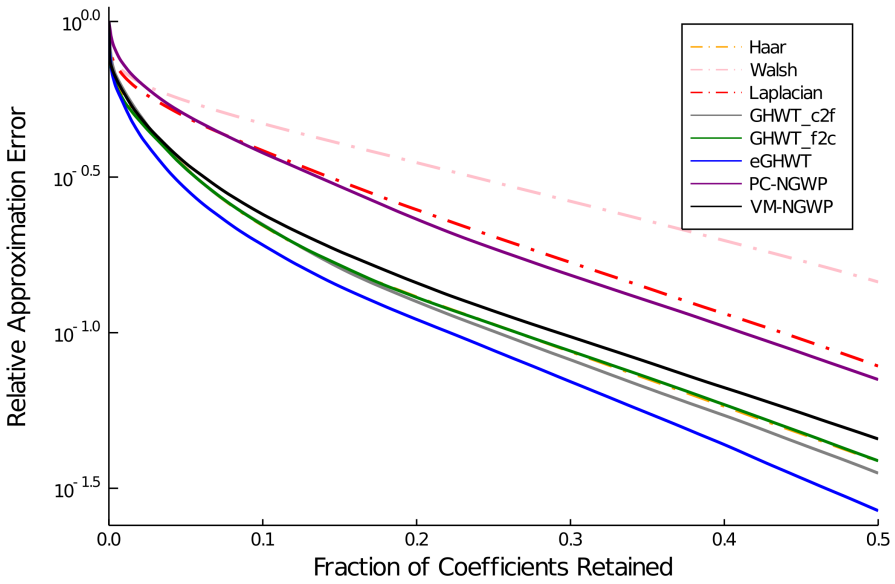

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Figure: (a) Pedestrian volume data in the city of Toronto; (b) Relative ℓ^2 approximation error of the data shown in (a) vs the fraction of kept coefficients.

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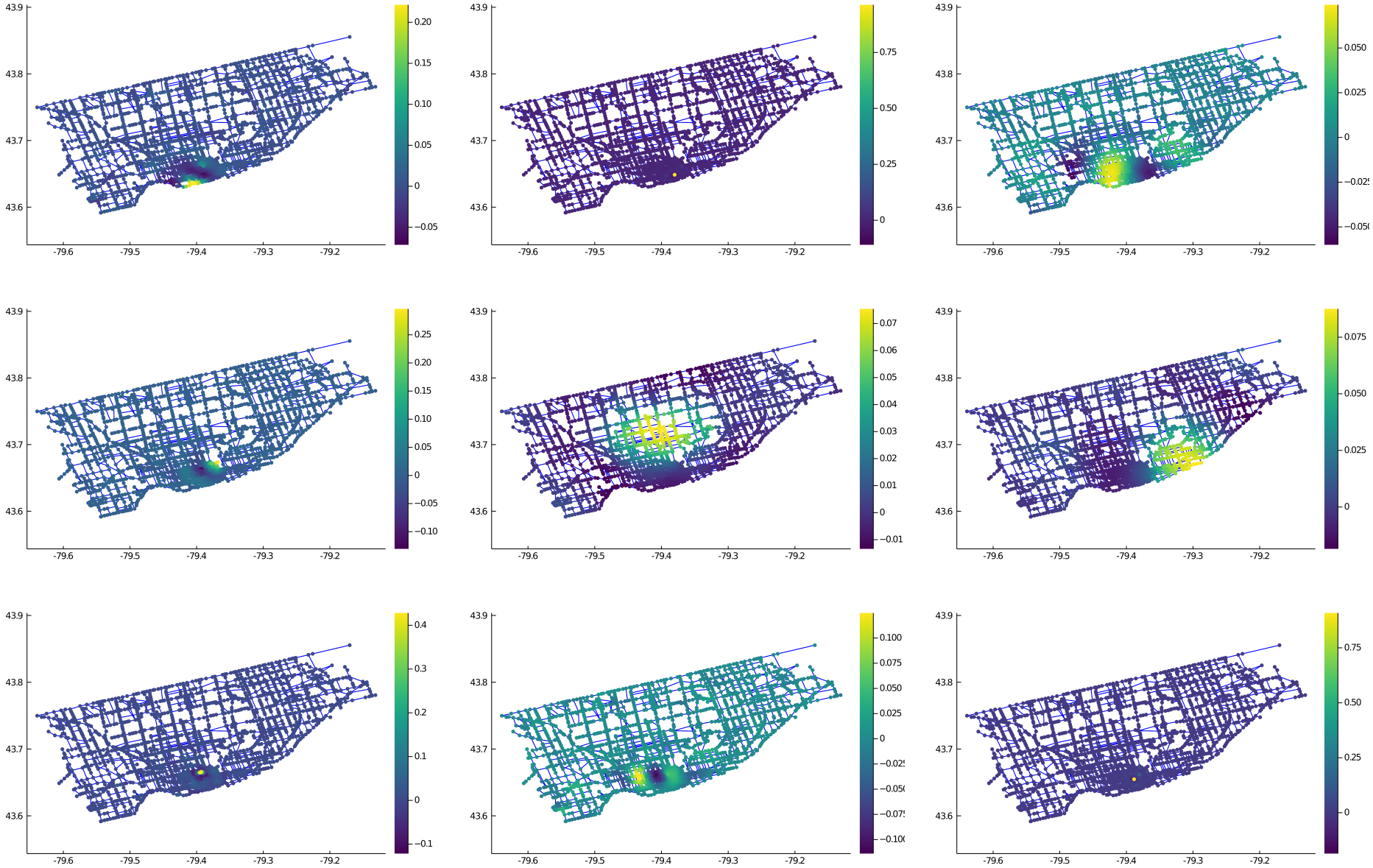

Observations from Examples 1 & 2

- Basis vectors that behave like *oriented edge detectors* are *automatically generated* in the NGWP dictionary.
- NGWP outperformed the other dictionaries on piecewise smooth graph signals
- NGWP performed reasonably well for graph signals sampled on an image containing oriented anisotropic texture patterns (e.g., Barbara's pants)
- NGWP was beaten by the eGHWT on the non-smooth and localized graph signal (e.g., pedestrian volume data on the Toronto street map)
- Potential reason I: NGWP is a direct generalization of the *Shannon* wavelet packet dictionaries, i.e., their "frequency" domain support is localized and well controlled while the "time" domain support is not compact.
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- Used the *hierarchical bipartitioning* of the dual $G^\star$ consisting of the GL eigenvectors as its nodes
- Used *varimax rotation* to get wavelet packet vectors well-localized on G.
- How to reduce computational complexity of $O(n^3)$
- How to proceed more precise approximation theoretic statements
- How to deal with the GL eigenvectors corresponds to *multiple eigenvalues*
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References

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Thank you very much for your attention!