Hierarchical Graph Laplacian Eigen Transforms

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2. Basics of Graph Laplacians
3. Hierarchical Graph Laplacian Eigen Transform (HGLET)
   - HGLET Variation: Generalized Haar Transform (GHT)
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Aims & Objectives

Wavelets

- Successful on regular domains
- Extend to irregular domains ⇒ "2nd Generation Wavelets"

For example:

- Hammond, Vandergheynst, and Gribonval (2011): wavelets via spectral graph theory
- Coifman and Maggioni (2006): diffusion wavelets
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Key difficulty: graphs lack the notion of *frequency*!

Common strategy: develop wavelet-*like* multiscale transforms

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Step 2. Investigate usefulness for:

1. Approximation/Denoising.
   - Smoothing crime rate data
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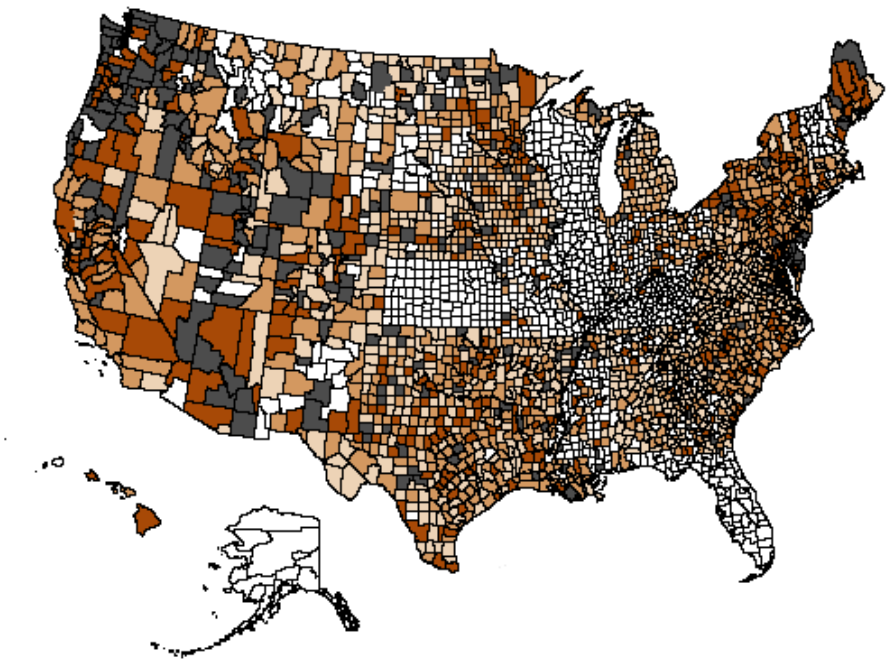

https://www.ncjrs.gov

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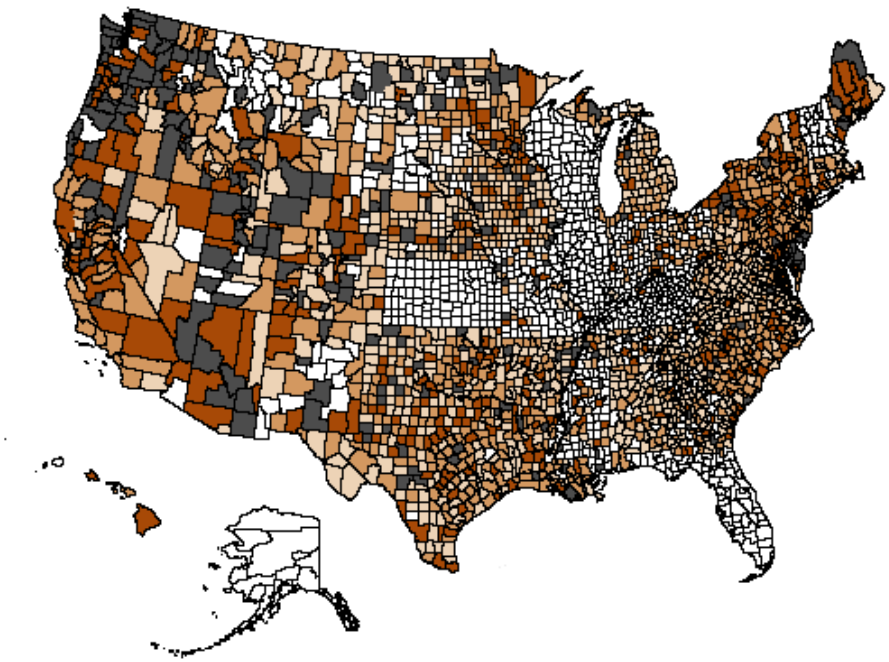

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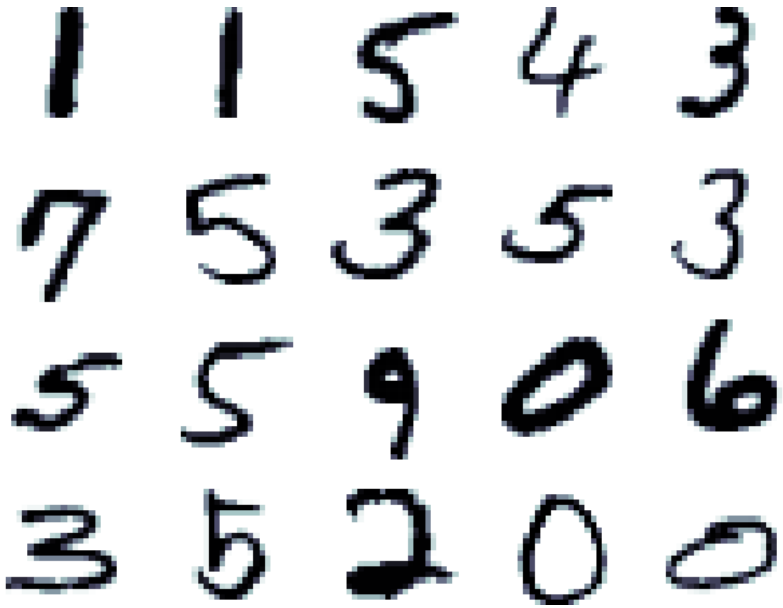
2. **Classification.**
   - Handwritten digit (MNIST) classification



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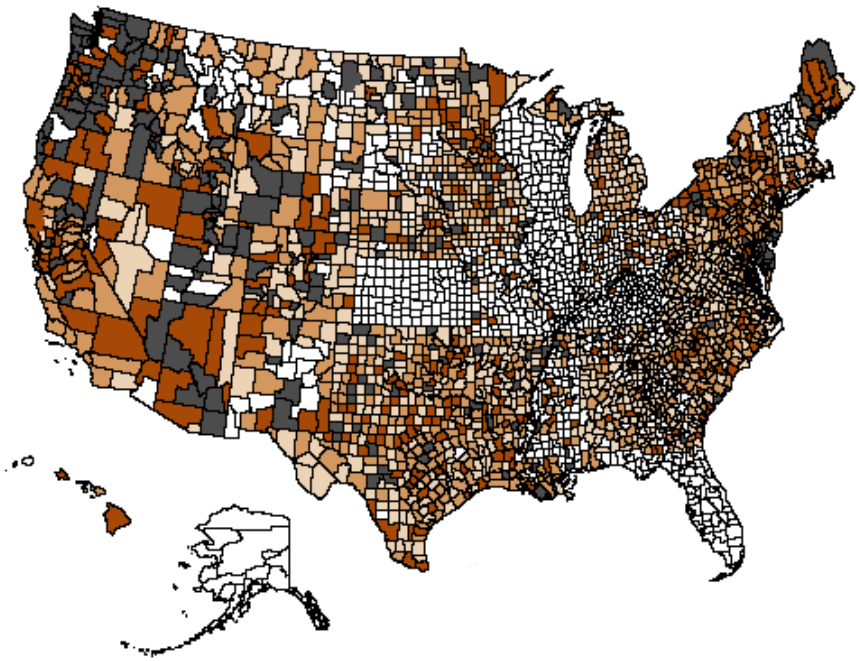

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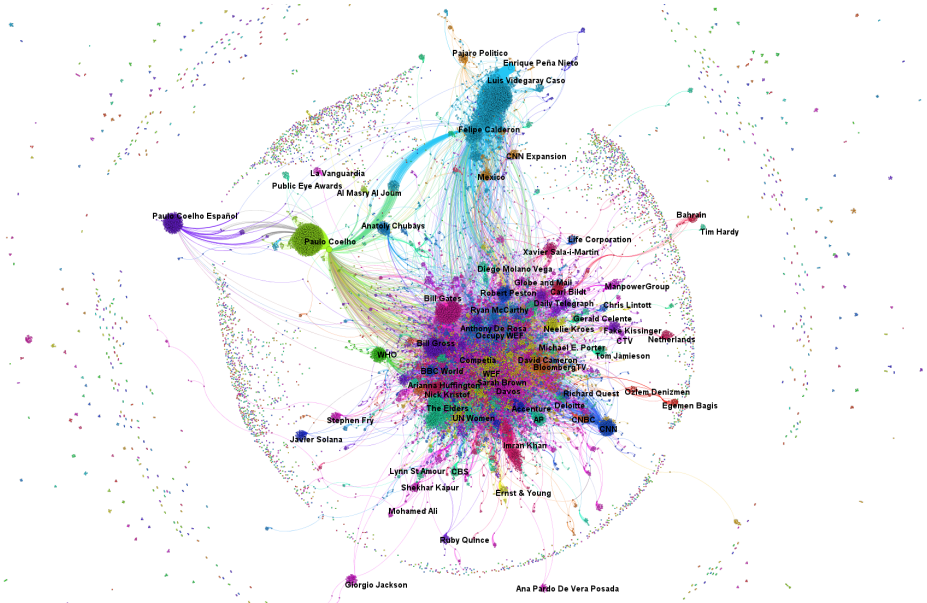
2. **Classification.**
   - Twitter spam classification/detection



http://beautifuldata.net

Basic Definitions and Notation

Consider a graph G.

- $V = V(G) = \{v_1, \ldots, v_N\}$ is the set of vertices
- $E = E(G) = \{e_1, \ldots, e_{N'}\}$ is the set of edges, where $e_k = (v_i, v_j)$ represents an edge (or line segment) connecting between adjacent vertices v_i, v_j for some $1 \leq i, j \leq N$
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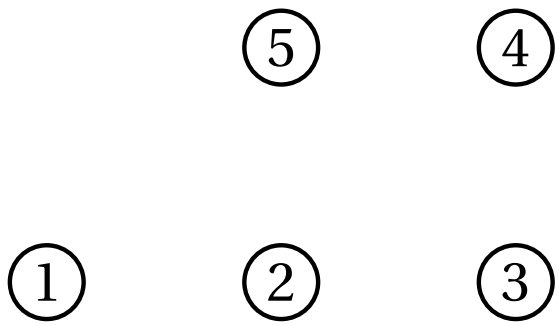

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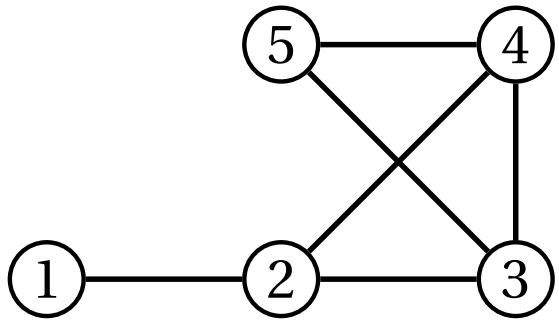

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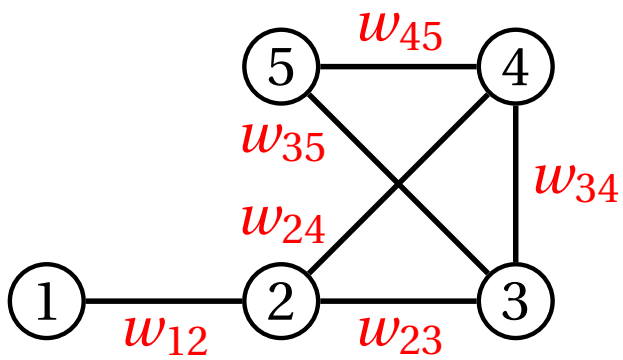

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Note that there are many ways to define w_{ij}.

For example, for *unweighted* graphs, we typically use

$$w_{ij} := \begin{cases} 1 & \text{if } v_i \sim v_j \text{ (i.e., } v_i \text{ and } v_j \text{ are adjacent);} \\ 0 & \text{otherwise.} \end{cases}$$

This is often referred to as the adjacency matrix and denoted by $A(G)$.

For *weighted* graphs, w_{ij} should reflect the similarity (or affinity) of information at v_i and v_j, e.g., if $v_i \sim v_j$, then

$$w_{ij} := 1/\mathrm{dist}(v_i, v_j) \quad \text{or} \quad \exp(-\mathrm{dist}(v_i, v_j)^2/\epsilon^2),$$

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Our Assumptions

We assume that the graph is

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- **undirected.** Edges do not have direction, which means that $w_{ij} = w_{ji}$ and thus W is symmetric.

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Graph Laplacians

$$\begin{cases} W(G) = (w_{ij}) & \text{the weight matrix} \\ D(G) := \operatorname{diag}(d_{v_1}, \ldots, d_{v_n}) & \text{the degree matrix, where } d_{v_i} := \sum_{j=1}^{N} w_{ij}. \\ L(G) := D(G) - W(G) & \text{the Laplacian matrix} \end{cases}$$

We also define the random walk Laplacian and symmetric normalized Laplacian matrices:

$$L_{\text{rw}}(G) := D^{-1}L = I - D^{-1}W$$
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Graph Laplacian Eigenvalues & Eigenvectors

$$L := D - W$$
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We have ($\diamondsuit$ denotes that it could refer to L, L_{rw}, or L_{sym}):

- sorted eigenvalues $0 = \lambda_0^{\diamondsuit} < \lambda_1^{\diamondsuit} \leq \cdots \leq \lambda_{N-1}^{\diamondsuit}$
- associated eigenvectors $\boldsymbol{\phi}_0^{\diamondsuit}$, $\boldsymbol{\phi}_1^{\diamondsuit}$, $\boldsymbol{\phi}_{N-1}^{\diamondsuit}$

The eigenvectors form a basis for $\mathbb{R}^N$. In particular:

- since L and L_{sym} are symmetric, their eigenvectors form orthonormal bases
- $\boldsymbol{\phi}_0 = \boldsymbol{\phi}_0^{\text{rw}} = \mathbf{1}/\sqrt{N}$
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Why Graph Laplacians?

- Let $f \in \mathbb{R}^N$. Then

$$Lf(v_i) = d_{v_i} f(v_i) - \sum_{j \neq i} w_{ij} f(v_j).$$

This is a generalization of *the finite difference approximation to the Laplace operator*.

- After all, *sines* (*cosines*) are the eigenfunctions of the Laplacian on the rectangular domain with Dirichlet (Neumann) boundary conditions.
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A Simple Yet Important Example: A Path Graph

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The eigenvectors of this matrix are exactly the *DCT Type II* basis vectors used for the JPEG image compression standard! (See e.g., Strang, SIAM Review, 1999).

- $\lambda_k = 2 - 2\cos(\pi k/N) = 4\sin^2(\pi k/2N),\ k = 0, 1, \ldots, N-1.$
- $\boldsymbol{\phi}_k(\ell) = \sqrt{2/N}\cos\left(\pi k(\ell + \frac{1}{2})/N\right),\ k, \ell = 0, 1, \ldots, N-1.$
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Now we turn our focus to a novel transform that can be viewed as a generalization of the block Discrete Cosine Transform. We refer to this transform as the Hierarchical Graph Laplacian Eigen Transform (HGLET).

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Graph Partitioning via Spectral Clustering

Goal: split the vertices V into two "good" subsets, X and X^c

Plan: use the signs of the entries in $\boldsymbol{\phi}_1$, which is known as the Fiedler vector

Why? Using $\boldsymbol{\phi}_1$ to generate X and X^c yields an approximate minimizer of the RatioCut function[1]:

$$\text{RatioCut}(X, X^c) := \frac{\text{cut}(X, X^c)}{|X|} + \frac{\text{cut}(X, X^c)}{|X^c|},$$

where

$$\text{cut}(X, X^c) := \sum_{\substack{v_i \in X \\ v_j \in X^c}} W_{ij}$$

[1] L. Hagen and A. B. Kahng: "New spectral methods for ratio cut partitioning and clustering," *IEEE Trans. Comput.-Aided Des.*, vol. 11, no. 9, pp. 1074-1085, 1992.

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Instead of RatioCut, we could consider the Normalized Cut function[1]:

$$\mathrm{NCut}(X, X^c) := \frac{\mathrm{cut}(X, X^c)}{\mathrm{vol}(X)} + \frac{\mathrm{cut}(X, X^c)}{\mathrm{vol}(X^c)},$$

where

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$$\mathrm{vol}(X) := \sum_{v_i \in X} d_{v_i}$$

Like before, an approximate solution is given by using the sign of $\boldsymbol{\phi}_1^{\mathrm{rw}}$ (or equivalently, $\boldsymbol{\phi}_1^{\mathrm{sym}} = D^{1/2}\boldsymbol{\phi}_1^{\mathrm{rw}}$).

[1] J. Shi & J. Malik: "Normalized cuts and image segmentation", *IEEE Trans. Pattern Anal. Machine Intell.*, vol. 22, no. 8, pp. 888–905, 2000.

Example of Graph Partitioning

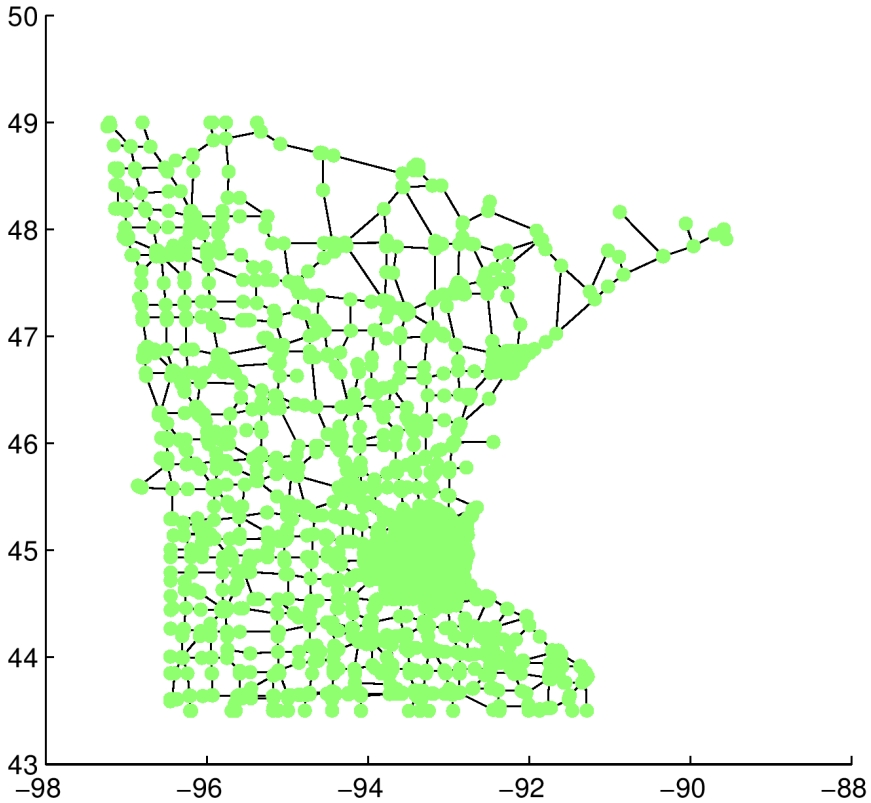

Figure: The MN road network

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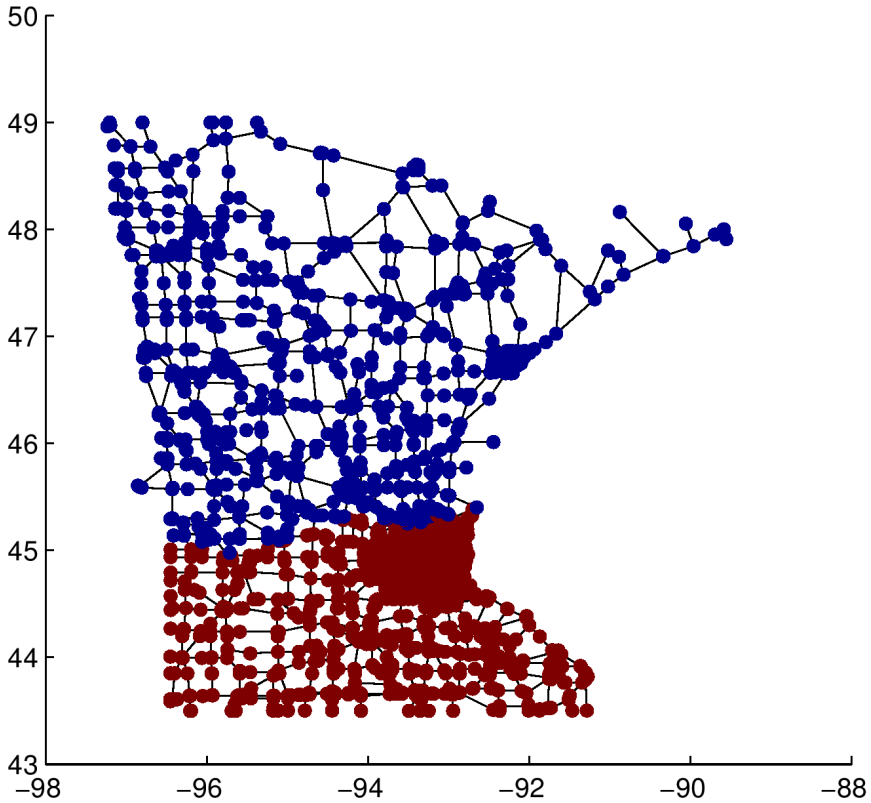

Figure: The MN road network partitioned via the Fiedler vector of L_{rw}

And now, we present our Hierarchical Graph Laplacian Eigen Transform:

1. Generate an orthonormal basis for the entire graph $\Rightarrow$ Laplacian eigenvectors (Notation is $\boldsymbol{\phi}_{k,l}^{j}$ with $j=0$)
2. Partition the graph using the Fiedler vector $\boldsymbol{\phi}_{k,1}^{j}$
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$$\left[\begin{array}{ccccc} \boldsymbol{\phi}_{0,0}^{0} & \boldsymbol{\phi}_{0,1}^{0} & \boldsymbol{\phi}_{0,2}^{0} & \cdots & \boldsymbol{\phi}_{0,N-1}^{0} \end{array} \right]$$

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Observations

- For an unweighted path graph, this yields a dictionary of the block DCT-II
- Similar to wavelet packet or local cosine dictionaries in that it generates an *overcomplete basis* from which we can select a basis useful for the task at hand ⇒ best-basis algorithm, local discriminant basis algorithm, ...
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HGLET Basis Vectors on MN

Here we display some of the basis vectors generated by our HGLET scheme on the MN road network. (Note: $j = 0$ is the coarsest scale, $j = 14$ is the finest.)

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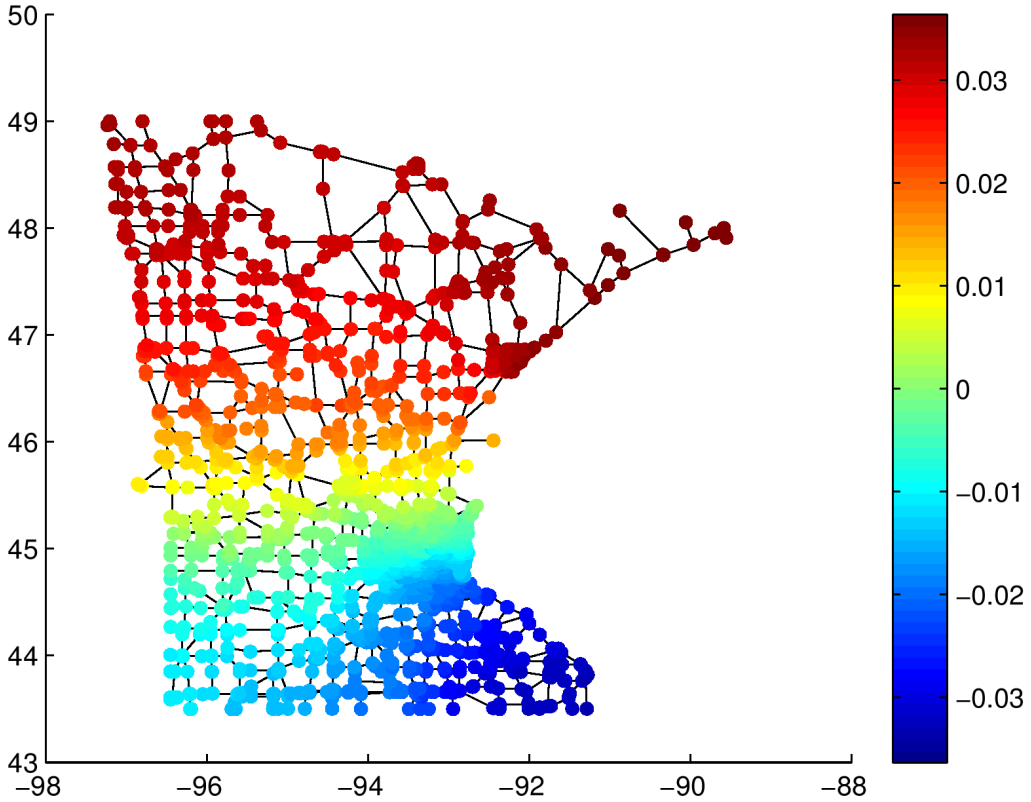

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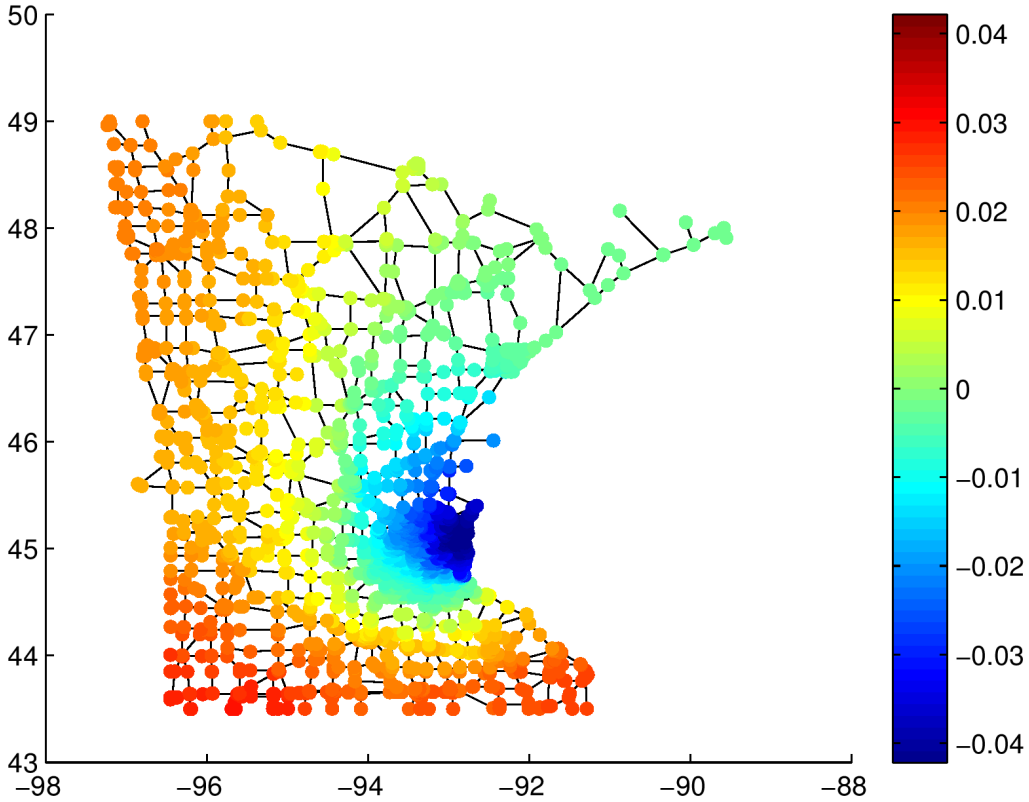

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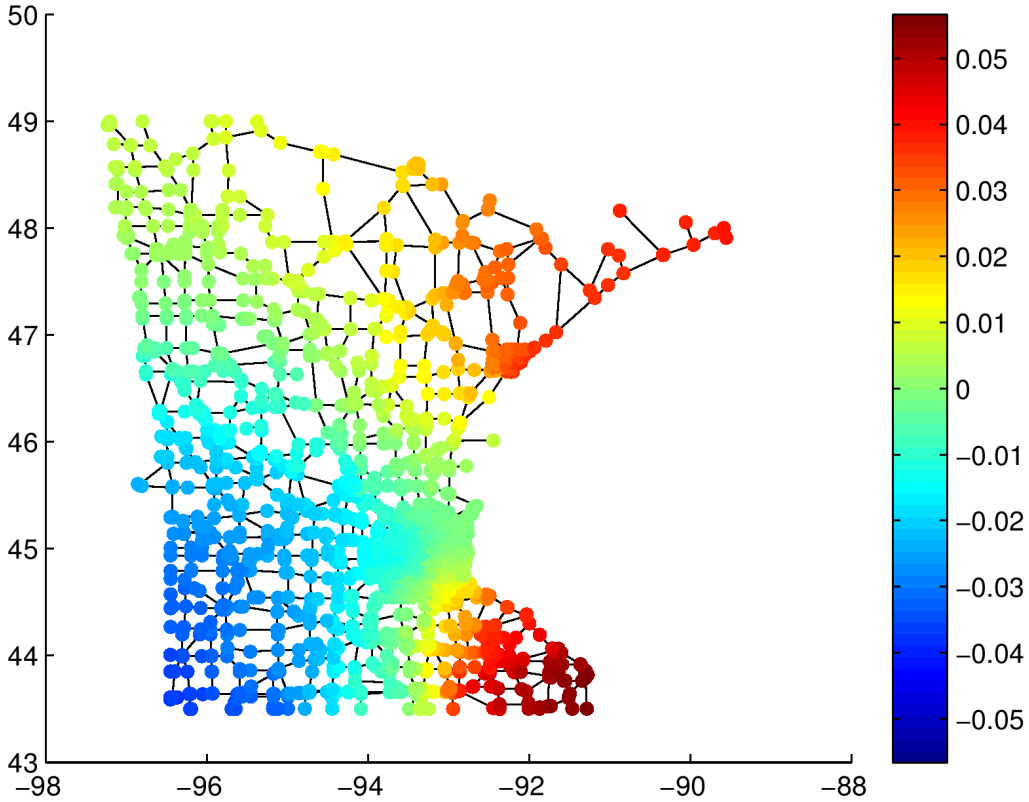

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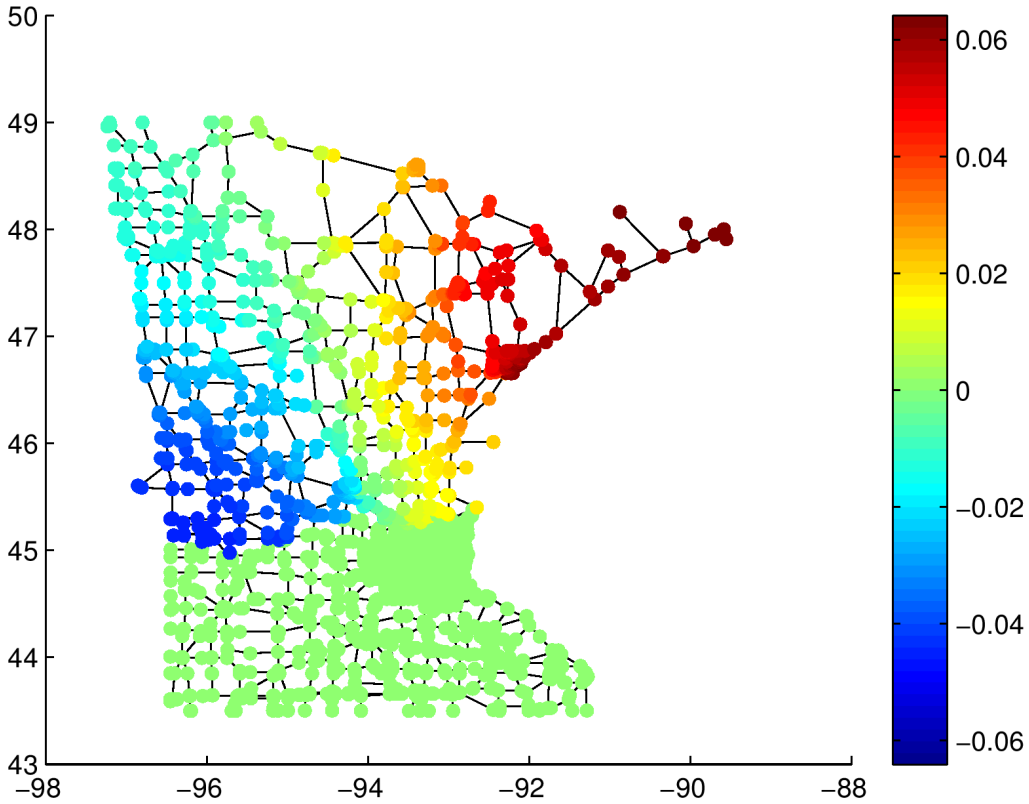

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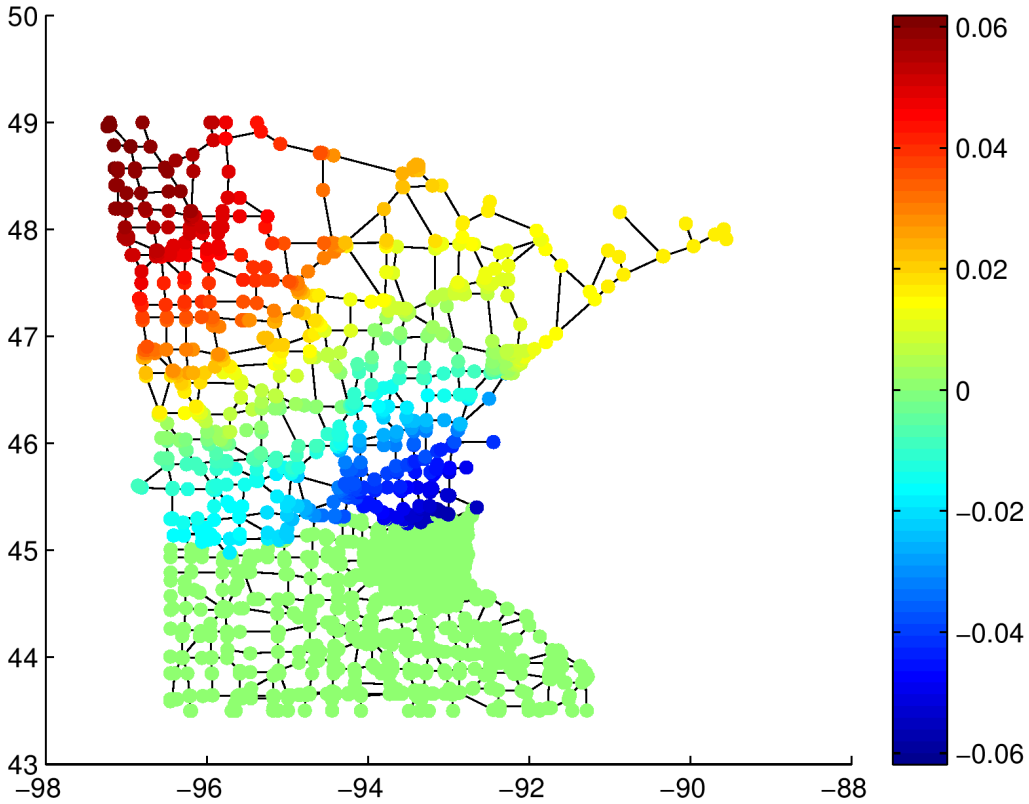

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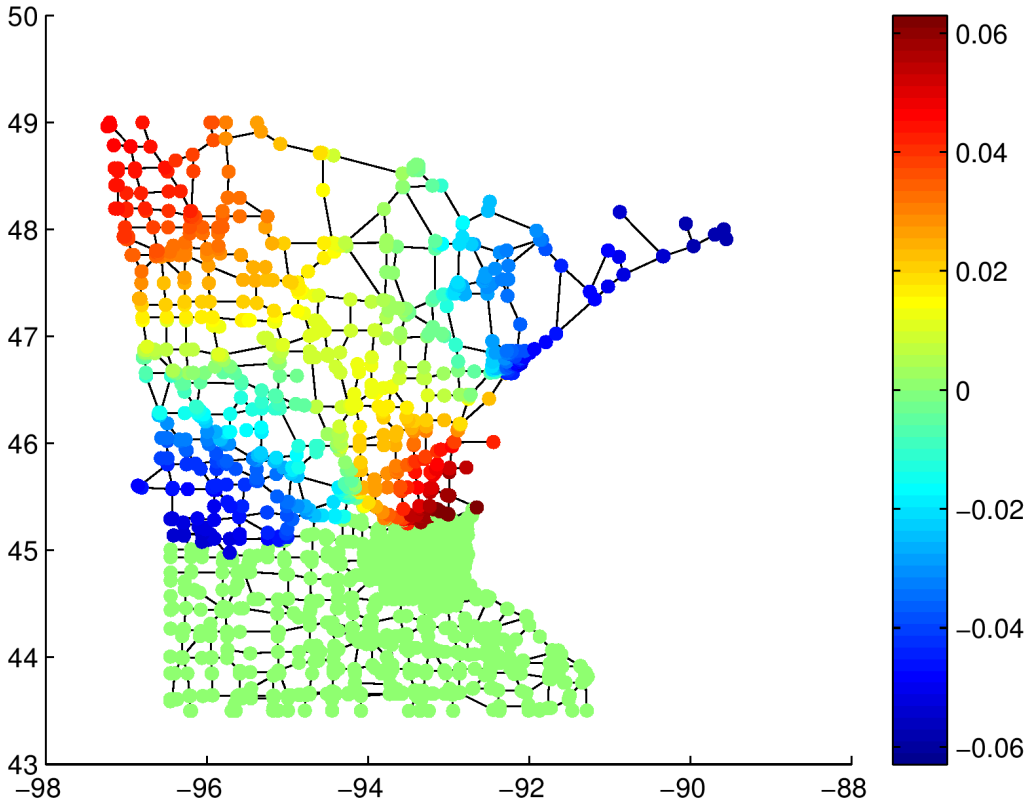

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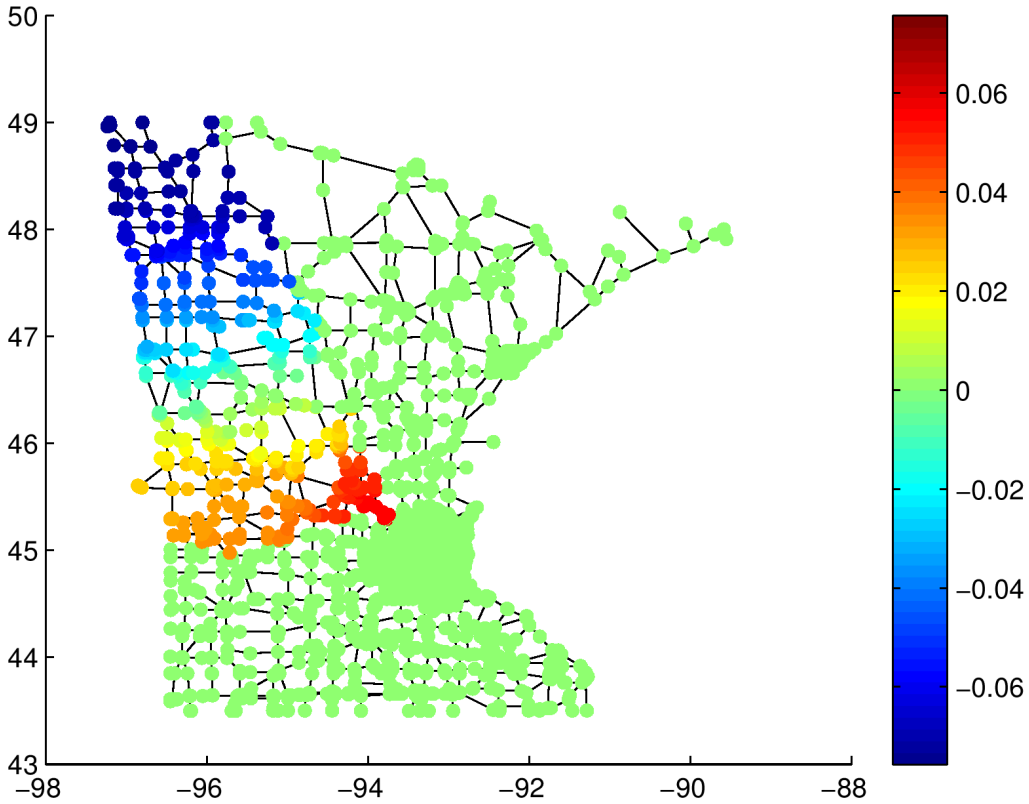

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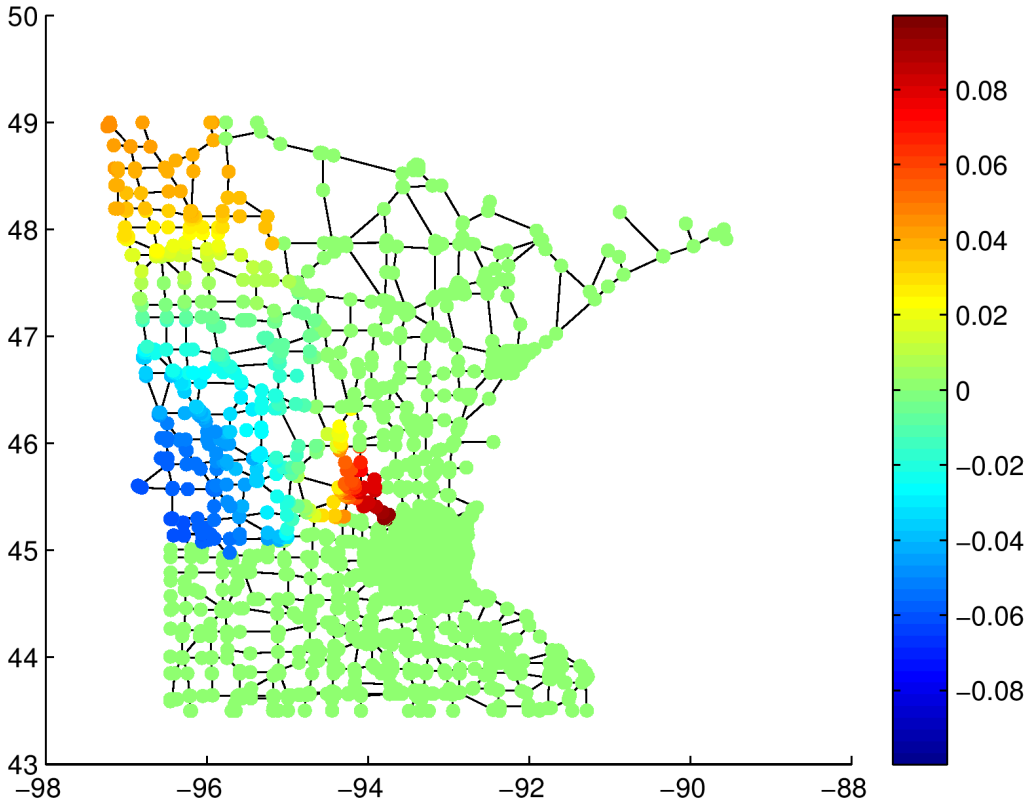

HGLET Basis Vectors on MN

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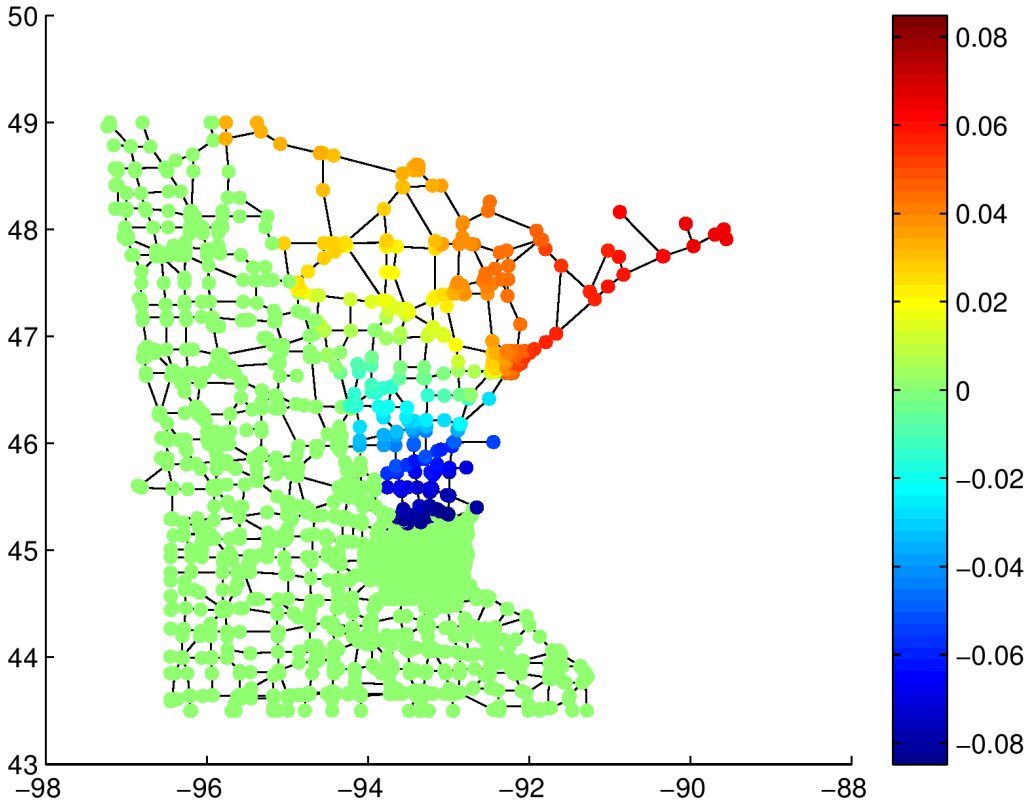

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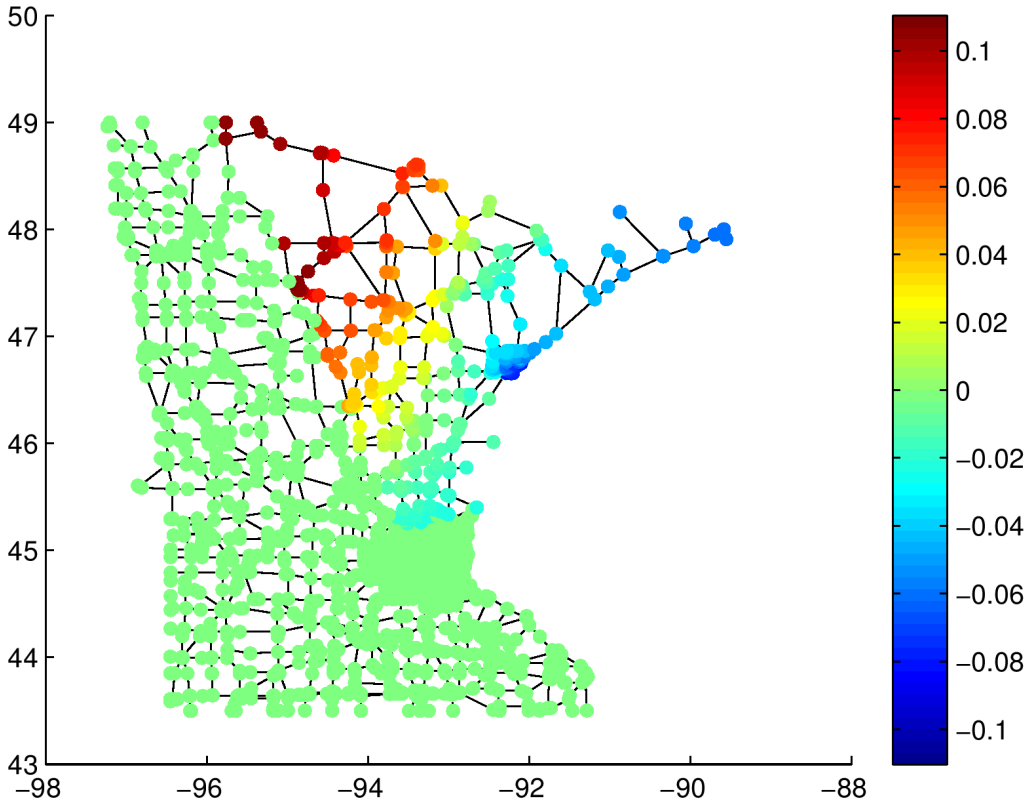

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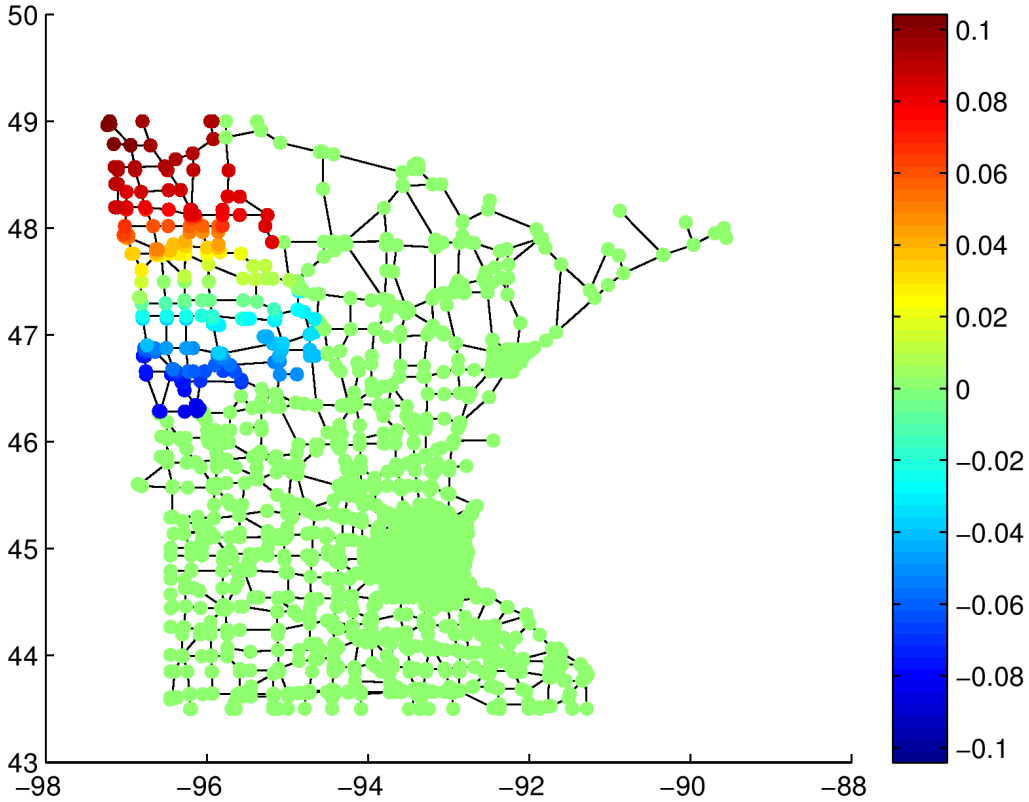

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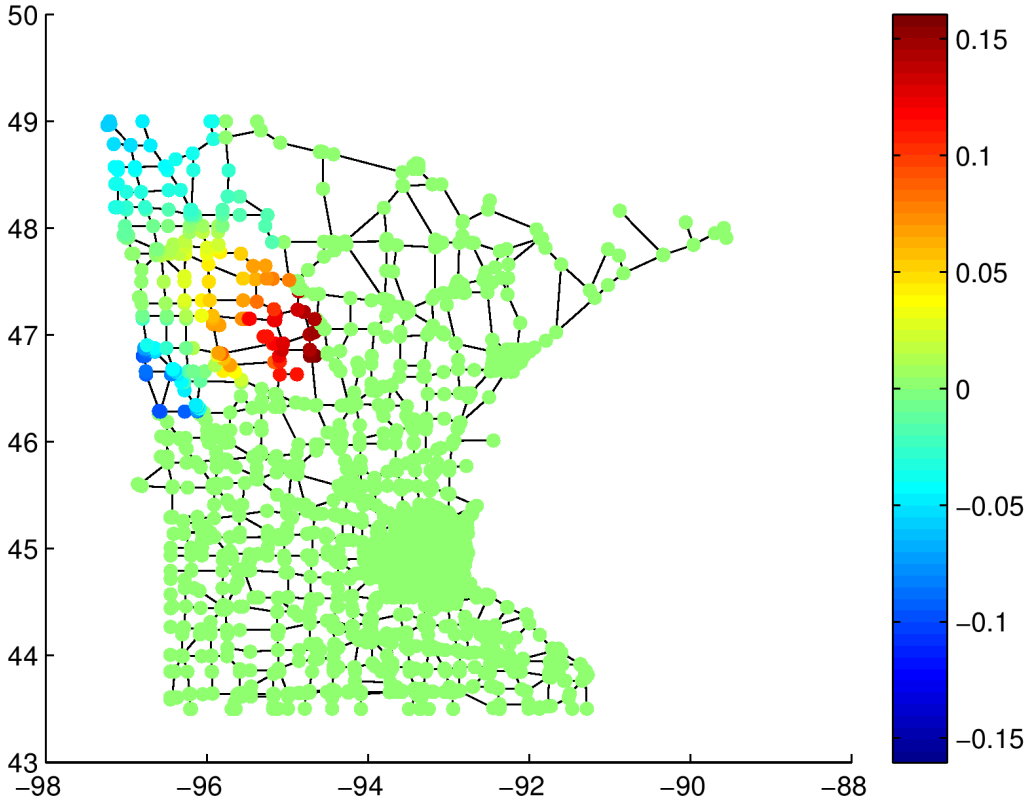

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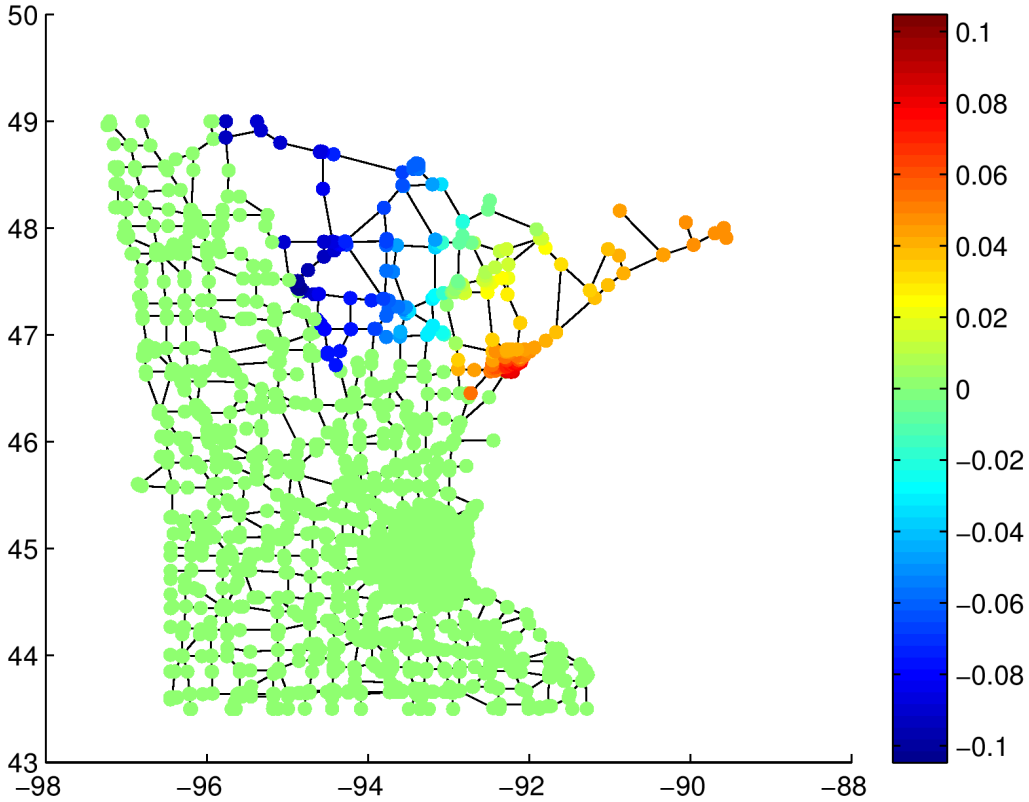

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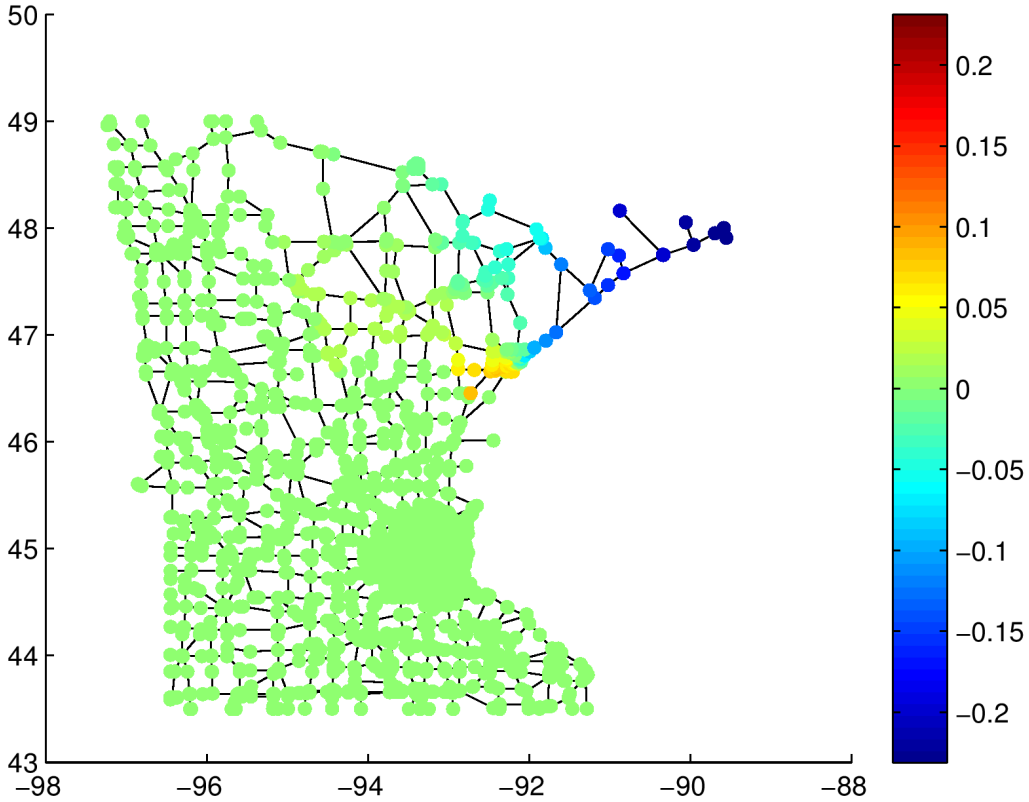

Computational Complexity: HGLET

	Computational Complexity	Run Time for MN[1]
HGLET (redundant)	$O(N^3)$	67 sec

[1] Computations performed on a personal laptop (4.00 GB RAM, 2.26 GHz), $N = 2640$ and $\texttt{nnz}(W) = 6604$.

Now we present a Haar-like modification of our scheme:

1. Starting with the entire graph (i.e., level $j = 0$), compute the Fiedler vector $\boldsymbol{\phi}_1$ ($\boldsymbol{\phi}_0$ is trivially known, and we denote it by $\varphi_{0,0}$). Convert $\boldsymbol{\phi}_1$ to a Haar-like vector:[1]

$$\psi_{0,0}(i) := \begin{cases} 1 & \text{if } \boldsymbol{\phi}_1(i) \geq 0 \\ -\frac{\#\text{ nonnegative}}{\#\text{ negative}} & \text{if } \boldsymbol{\phi}_1(i) < 0 \end{cases}$$

   and then ℓ^2-normalize it

2. Partition the graph $\Rightarrow$ Fiedler vector
3. Compute the Fiedler vector for each partition and convert it to a Haar-like vector on its respective partition[1] $\Rightarrow \psi_{j,k}$
4. Repeat...

This yields an orthonormal basis: $\varphi_{0,0} \cup \{\psi_{j,k}\}_{0 \leq j < J,\ k}$

[1] We have also developed a method that, like the HGLET, generates a full orthonormal basis on each each region at each level. The basis consists of piecewise-constant orthonormal vectors, similar to the *Walsh-Hadamard transform*.

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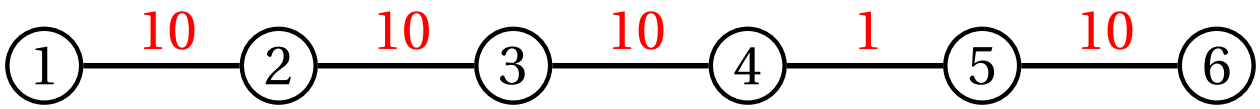

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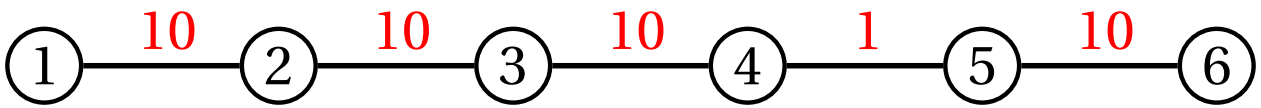

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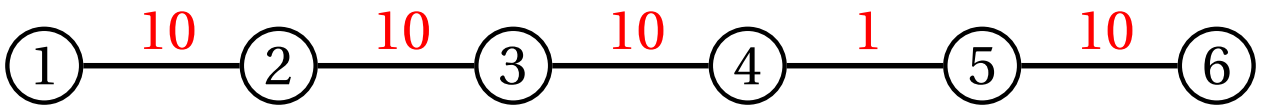

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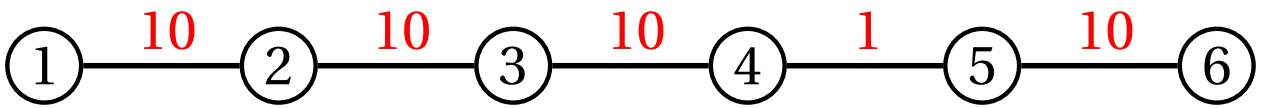

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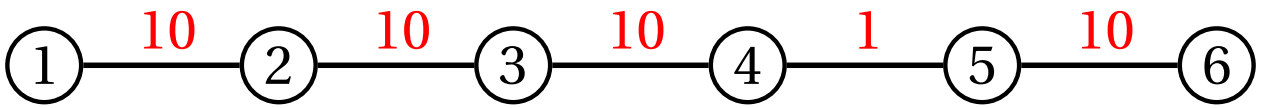

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Thus, we generate a matrix whose columns (after ℓ^2-normalization) form an orthonormal basis:

$\varphi_{0,0}$	$\psi_{0,0}$	$\psi_{1,0}$	$\psi_{1,1}$	$\psi_{2,0}$	$\psi_{2,1}$
1	1	1	0	1	0
1	1	1	0	−1	0
1	1	−1	0	0	1
1	1	−1	0	0	−1
1	−2	0	1	0	0
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Computational Complexity: GHT

	Computational Complexity	Run Time for MN[1]
HGLET (redundant)	$O(N^3)$	67 sec
GHT	$O(N \log N)$	4 sec

[1] Computations performed on a personal laptop (4.00 GB RAM, 2.26 GHz), $N = 2640$ and $\mathtt{nnz}(W) = 6604$.

Coifman and Wickerhauser (1992) developed the best-basis algorithm as a means of selecting the basis from a dictionary of wavelet packets that is best for approximation/compression.

We generalize this approach, developing and implementing an algorithm for selecting the basis from the dictionary of HGLET bases that is best for approximation.

As before, we require a cost functional $\mathscr{J}$. For example:

$$\mathscr{J}(\boldsymbol{x}) = \left(\sum_{i=1}^{n} |x_i|^p \right)^{1/p} = \texttt{norm(x,p)}$$

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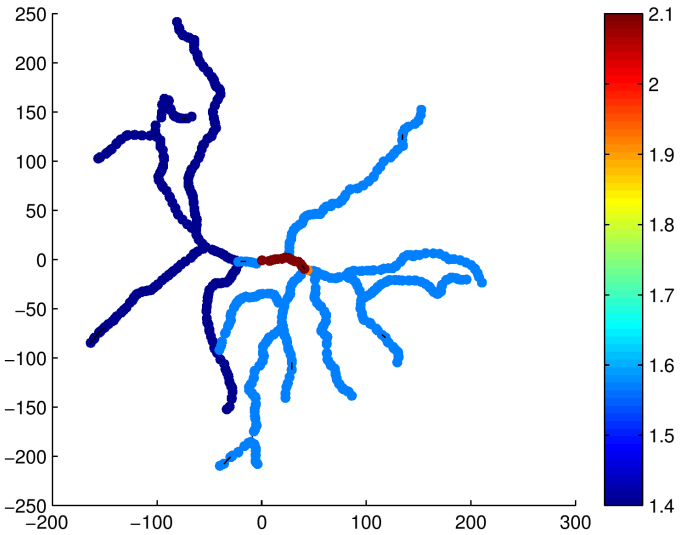
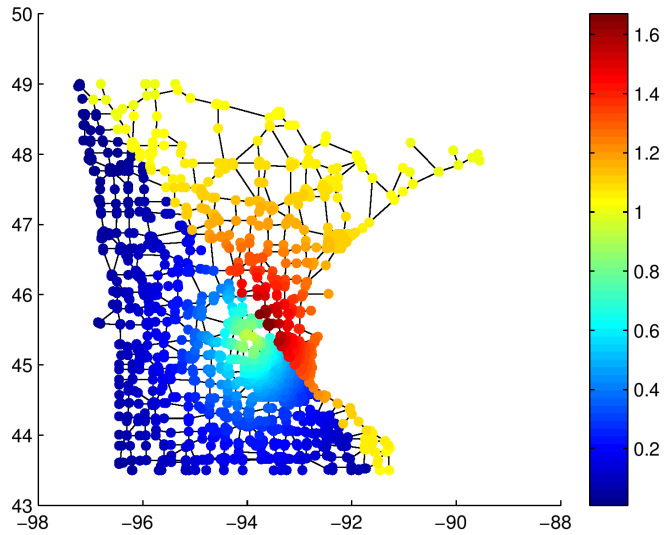
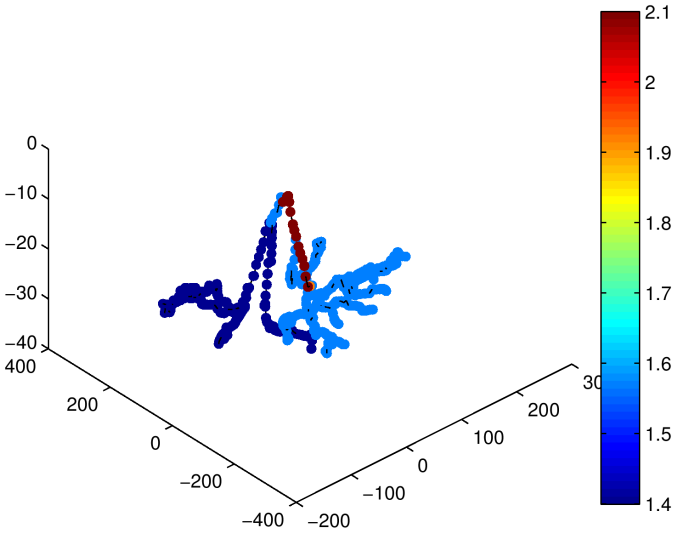
According to cost functional $\mathscr{J}$, this is the best basis for approximation.



(a) Thickness data on a dendritic tree



(b) A mutilated Gaussian on the MN road network



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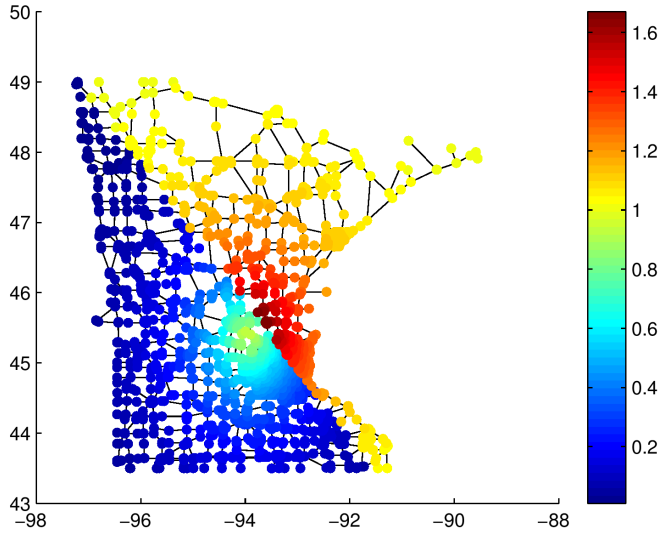

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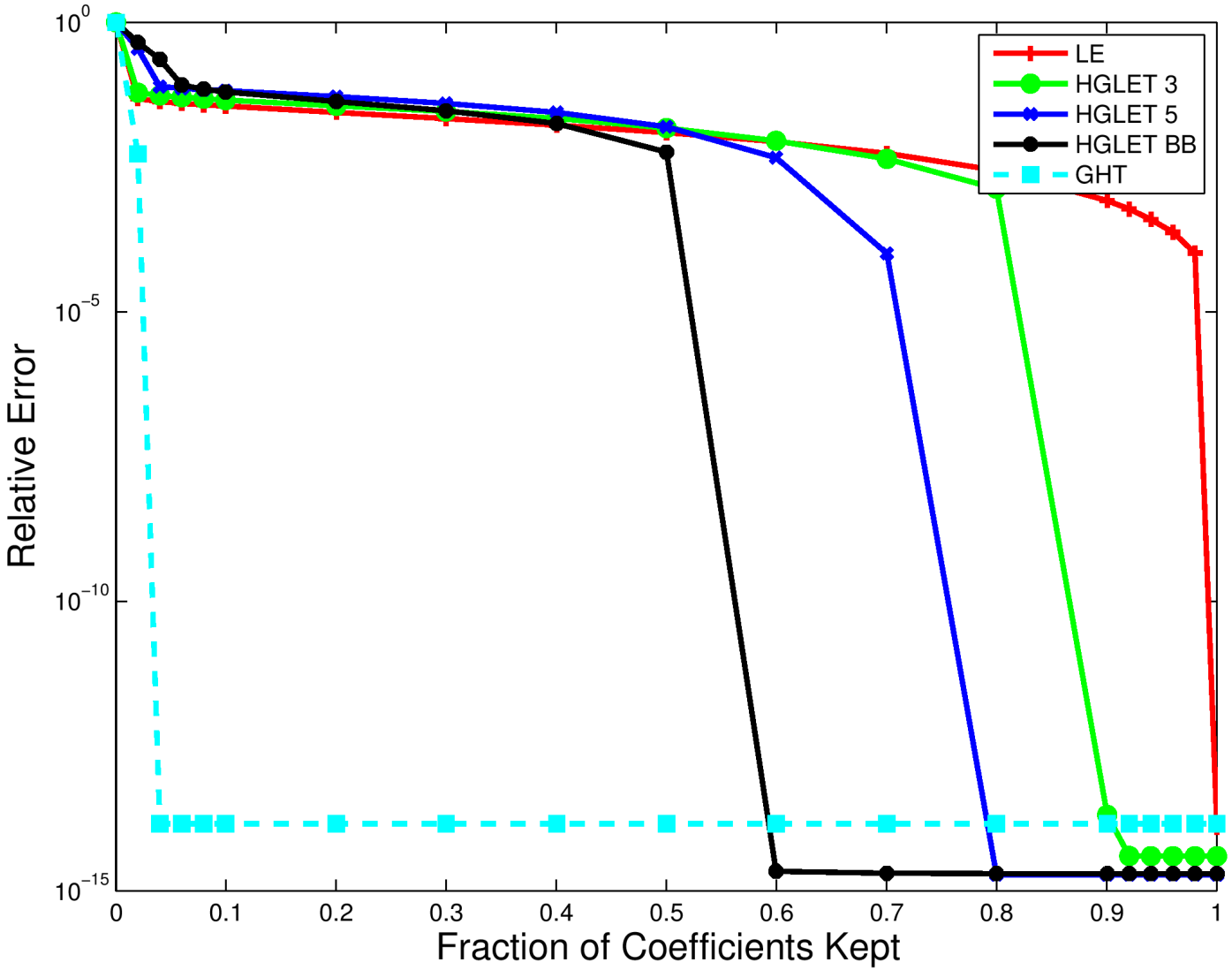
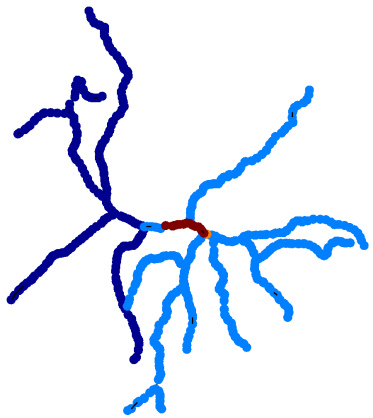
Dendrite (L_{rw}, adjacency matrix)





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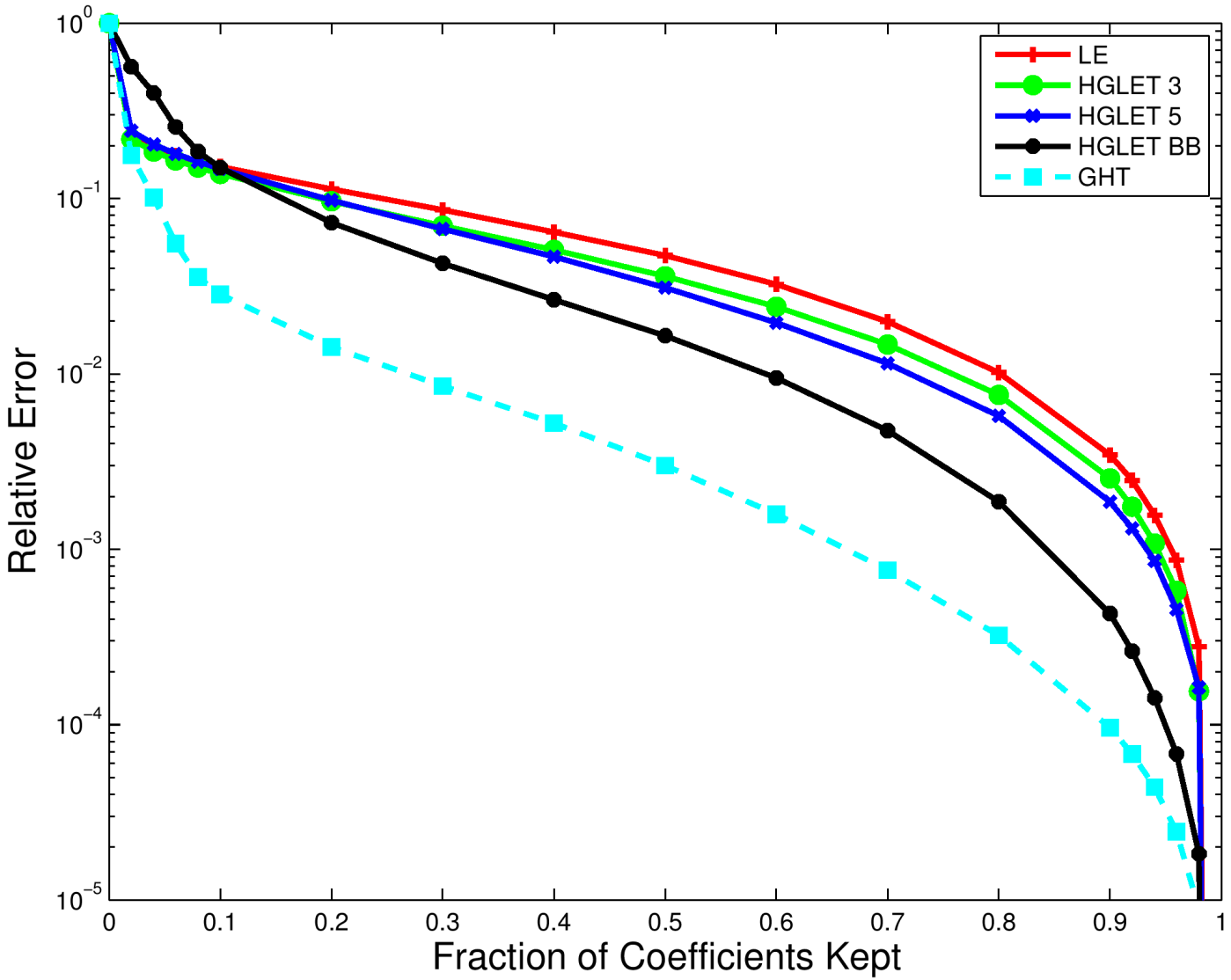
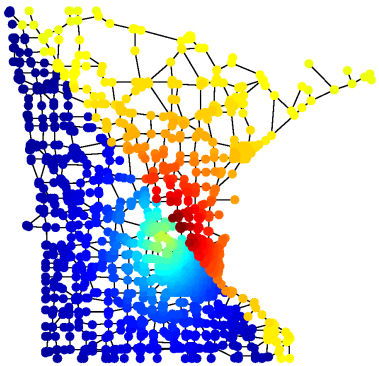
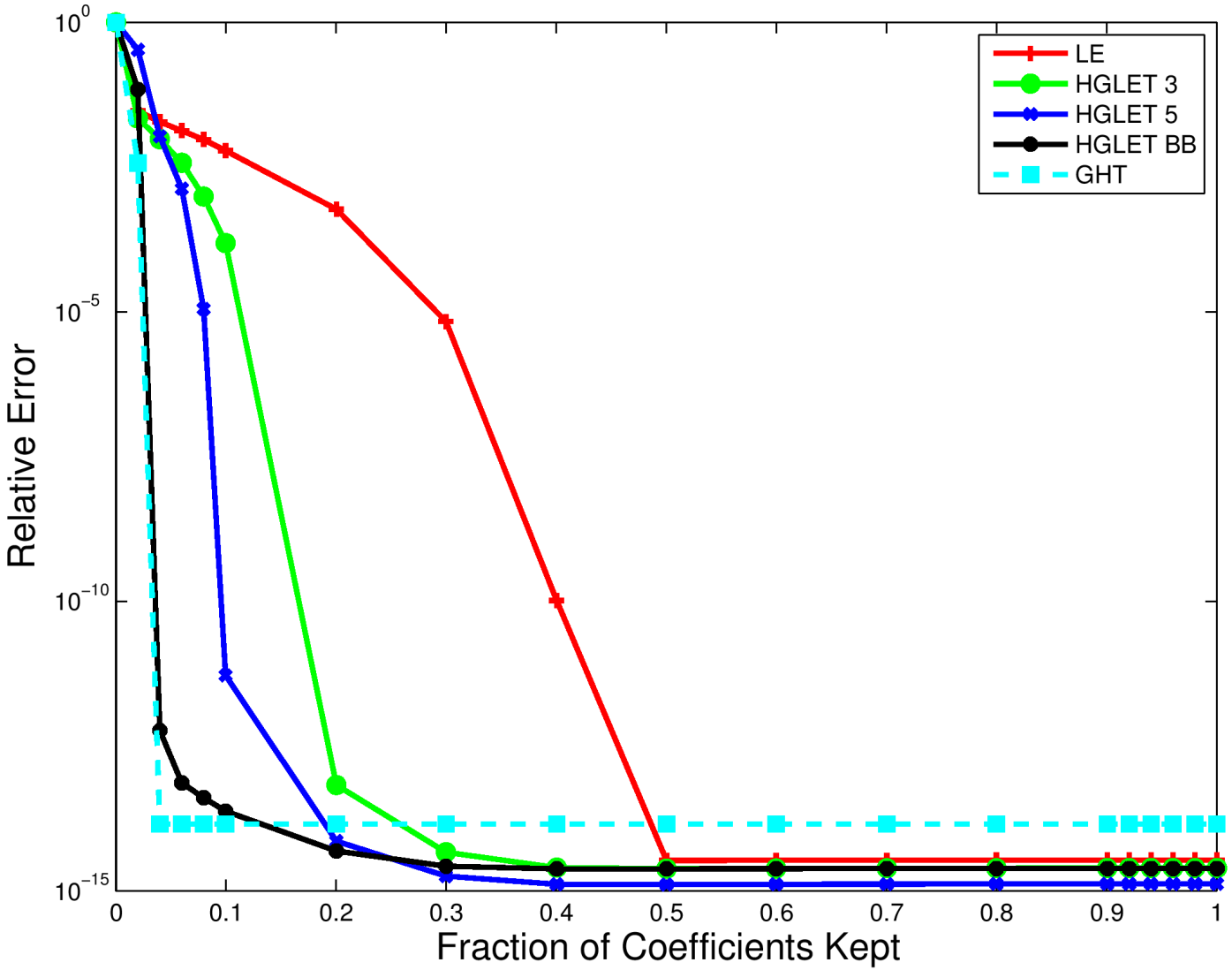
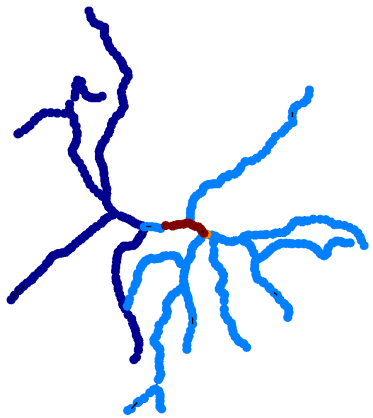




Dendrite (L, inverse Euclidean weights)





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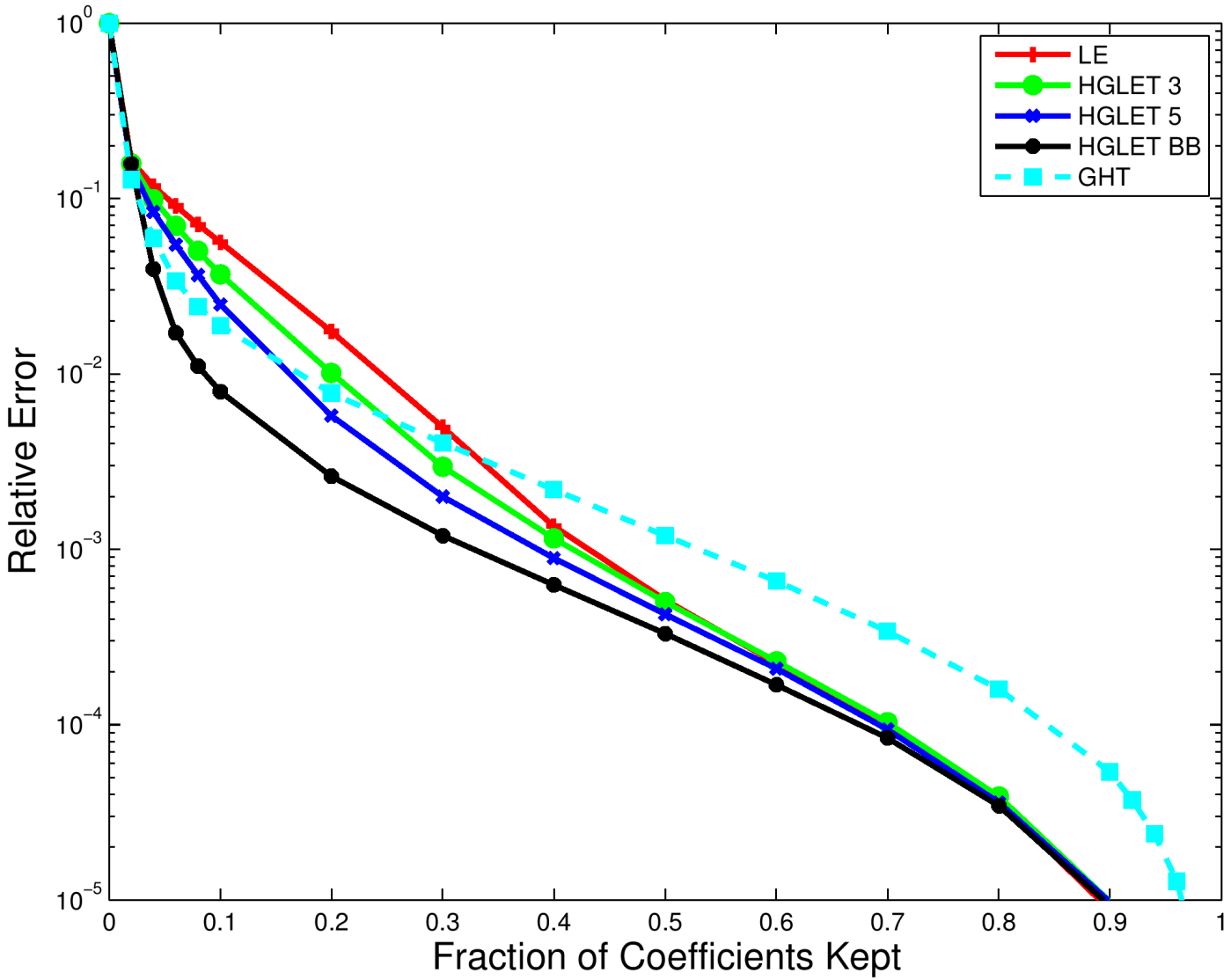

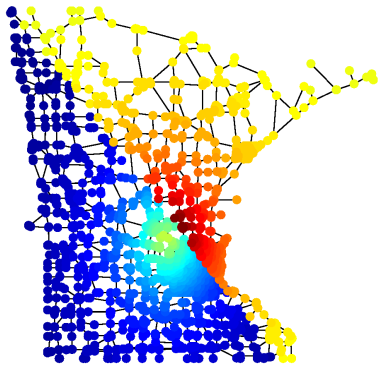

Discussion of Approximation Results

- Overall, we see that HGLET best-basis > HGLET Level 5 > HGLET Level 3 > Laplacian eigenvectors (HGLET Level 0)
  - This demonstrates the merit of using *localized basis vectors*.
- For all data sets, the best performer is either the GHT or the best-basis HGLET.
  - This makes a strong case for using localized basis vectors on *multiple scales*.
  - It's no surprise that the GHT is the best performer on the Dendrite data set.
  - How does the GHT compete on the smoother MN data set?
    - $\Rightarrow$ Its basis contains one Haar-like vector for *each and every region* in the hierarchical partitioning.

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  - Developing a *true* generalization of wavelet and wavelet packet transforms is more challenging due to the difficulty of the notion of the *frequency domain* of a given graph.
- The HGLET is a direct generalization of *Hierarchical Block Discrete Cosine Transforms* originally developed for regularly-sampled signals and images.
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Future Work

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References & Acknowledgments

- http://www.math.ucdavis.edu/~saito/courses/HarmGraph/ contains Naoki Saito's course slides and useful information on "Harmonic Analysis on Graphs and Networks"
- Also visit http://www.math.ucdavis.edu/~saito/publications/ for various related publications including:
  - N. Saito: "Data analysis and representation using eigenfunctions of Laplacian on a general domain," *Applied & Computational Harmonic Analysis*, vol. 25, no. 1, pp. 68–97, 2008.
  - N. Saito & E. Woei: "Analysis of neuronal dendrite patterns using eigenvalues of graph Laplacians," *Japan SIAM Letters*, vol. 1, pp. 13–16, 2009.
  - J. Irion & N. Saito: "Hierarchical graph Laplacian eigen transforms," submitted for publication, 2013.

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