# Exploiting Data-Dependent Structure for Improving Sensor Acquisition and Integration

#### Alexander Cloninger

Norbert Wiener Center Department of Mathematics University of Maryland, College Park http://www.norbertwiener.umd.edu

#### April 14, 2014



#### Outline



- 2 Characterizing Embeddings for Disjoint Graphs
- Eigenvector Localization of Graphs with Weakly Connected Clusters





#### Introduction to Thesis Research

Characterizing Embeddings for Disjoint Graphs Eigenvector Localization of Graphs with Weakly Connected Clusters Examples and Conclusions

#### Outline



#### Introduction to Thesis Research





#### **Data-Dependent Structure**

- Advancements in sensor construction and production cost has led to a deluge of data
- Thesis utilizes data-dependent operators to discover efficient representations of data
- This focus on learning structure splits into three topics
  - Building data-dependent graphs to capture structure and detect anomalous objects
  - Fusing low-dimensional parameters from heterogeneous data sources
  - Exploiting compressibility of data to reduce sampling requirements prior to collection

< □ > < 同 > < 回 > <

### Reduced Acquisition Time

- Based on the theory of compressive sensing and matrix completion
  - Recover signal that is sparse in some basis
  - Key is that measurements are randomly made and *incoherent* with respect to sparsity basis
  - Utilizes convex relaxation and optimization schemes to reconstruct signal
  - Reconstruction only requires O (K log N) measurements

#### **Contributions of Thesis**

- Proved *bounded norm Parseval frames* satisfy necessary conditions for matrix reconstruction
- Demonstrated use of matrix completion for solving 2D Fredholm integrals from incomplete measurements
- Improved acquisition time for nuclear magnetic resonance spectroscopy via reducing necessary number of samples

Center

# Fusing Low Dimensional Parameters of High Dimensional Data

- Based on graph and operator theoretic approaches to pattern recognition and machine learning
  - Builds operator that encodes similarity between data points
  - Takes data from high-dimensional data space and embeds into low-dimensional euclidean space
  - Allows common comparison across heterogeneous sensors

#### **Contributions of Thesis**

- Built approximate inversion algorithm for Laplacian eigenmaps that utilizes compressive sensing
- Used inversion along with Coifman and Hirn's graph rotation to create data fusion algorithm
- Reconstructed missing LIDAR data (altitudes) from hyperspectral camera images (electromagnetic spectrum frequencies)

Center plications

### Laplacian Eigenmaps

- Let  $\Omega = \{x_1, ... x_n\} \subset \mathbb{R}^d$  be a set of data points, or *data space*
- Idea is to learn structure via inter-data similarities
- Encode relationships via symmetric kernel  $k : \Omega \times \Omega \rightarrow [0, 1]$ 
  - Gaussian kernel,  $k(x, y) = e^{-\frac{\|x-y\|_2^2}{2\sigma^2}}$
  - Mahalanobis distance,  $k(x, y) = e^{-(x-y)^T S^{-1}(x-y)}$
  - Graph adjacency,  $k(x, y) = \begin{cases} 1 & : x \in \mathcal{N}(y), \\ 0 & : \text{ otherwise.} \end{cases}$
- Build graph  $G = (\Omega, E, W)$ , where  $\{x, y\} \in E \iff k(x, y) \approx 1$

イロト イポト イヨト イヨト

- $W_{x,y} = k(x, y)$  if  $\{x, y\} \in E$
- k-Nearest Neighbors
- Key is that G is sparse

#### Laplacian Eigenmaps (cont.)

- Calculate the normalized graph Laplacian  $L = I D^{-1/2} W D^{-1/2}$ , where  $D_{x,x} = \sum_{y} W_{x,y}$
- Solve the eigenvalue problem

$$L\phi_i = \lambda_i \phi_i$$

• 
$$0 = \lambda_0 \le \lambda_1 \le ... \le \lambda_{n-1} \le 2$$
  
•  $\langle \phi_i, \phi_j \rangle = 0$  for  $i \ne j$ 

#### LE Embedding

$$\Phi : \Omega \to \mathbb{R}^m x \mapsto [\phi_1(x), ..., \phi_m(x)]$$

Forms low dimensional embedding that preserves local neighborhood structure

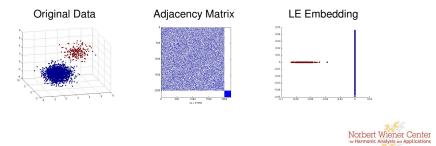
• Minimizes 
$$\sum_{x,y} \|\Phi(x) - \Phi(y)\| \frac{W_{x,y}}{\sqrt{D_{x,x}D_{y,y}}}$$

#### Graph Representation of Data Set

 Maps points from complicated data space to Euclidean feature space

• 
$$D_{LE}(x, y) = \|\Phi(x) - \Phi(y)\|_2$$

• Can be used to reduce dimension of data



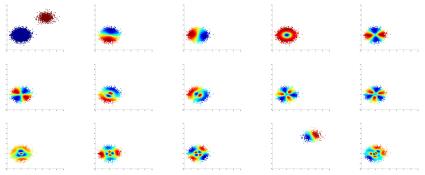
< □ > < 同 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □

# Complicated Distribution of Eigenvectors

- Most literature simply utilizes "first *m* eigenvectors with non-zero eigenvalue"
  - These correspond to "low frequency" information on graph
- When in doubt, simply be liberal with choice of m
- However, distribution of eigenvectors more complicated
  - Do not simply correspond to 1 eigenvector concentrated on each cluster
- Rest of talk is examination of eigenvector localization and order of emergence
  - Specifically when clusters are differing sizes

### Examples of Small Clusters Failing to Emerge

#### Eigenvectors with non-zero eigenvalues



 $|C_1| = 10,000, |C_2| = 1,000$ 



#### Introduction to Thesis Research

Characterizing Embeddings for Disjoint Graphs Eigenvector Localization of Graphs with Weakly Connected Clusters Examples and Conclusions

# **Outline of Approach**

- Assume graph G = (Ω, E) already formed from data, under some metric and using k-NN
- For simplicity, assume  $\{x, y\} \in E \iff y \in \mathcal{N}(x)$  and  $w_{x,y} = 1$ 
  - Approximates behavior of LE while utilizing vast literature on regular graph
- Wish to examine emergence of small clusters in eigenvectors
- Approach:
  - Characterize eigenpairs of disjoint graphs with heterogeneous sized clusters
  - Demonstrate that, upon adding edges to connect graph, eigenpairs do not deviate far from those of disjoint graph

(日)

#### Introduction to Thesis Research

Characterizing Embeddings for Disjoint Graphs Eigenvector Localization of Graphs with Weakly Connected Clusters Examples and Conclusions

# **Outline of Approach**

- Assume graph G = (Ω, E) already formed from data, under some metric and using k-NN
- For simplicity, assume  $\{x, y\} \in E \iff y \in \mathcal{N}(x)$  and  $w_{x,y} = 1$ 
  - Approximates behavior of LE while utilizing vast literature on regular graph
- Wish to examine emergence of small clusters in eigenvectors
- Approach:
  - Characterize eigenpairs of disjoint graphs with heterogeneous sized clusters
  - Oemonstrate that, upon adding edges to connect graph, eigenpairs do not deviate far from those of disjoint graph

(日)

#### Outline



#### 2 Characterizing Embeddings for Disjoint Graphs

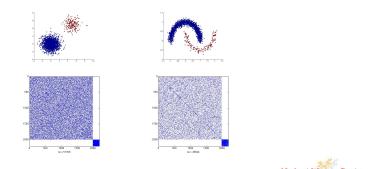
Eigenvector Localization of Graphs with Weakly Connected Clusters





# Similarity of Data Generated Graphs

- By analyzing graph, can bypass specifics of data set
- Characteristics such as convexity and scale can be ignored



< < >> < </p>

### **Clusters as Regular Graphs**

- Need way to characterize data clusters
- Define data cluster on *n* nodes to be random regular graph

#### Definition (Family of Regular Graphs)

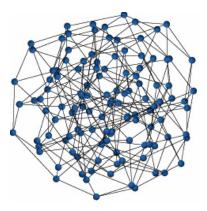
The family of regular graphs  $\mathcal{G}_{n,k}$  is the set of all graphs G = (V, E) such that:

V contains n nodes

$$\forall x \in V, \deg(x) \equiv |\{y \in V : \{x, y\} \in E\}| = k.$$

- Random regular graph is  $G \in \mathcal{G}_{n,k}$  chosen uniformly at random from all graphs
- With high probability, G does not have large cycles or large complete subgraphs

### Random Regular Graphs



Donetti, Neri, and Muño 2006



# Validity of Regular Graph Assumption

- Ties into k-Nearest Neighbors edges for graph
- If ignoring need for weights to be symmetric, then exactly generates k-regular graph
- Following theory also applies for Erdös Renyi graph

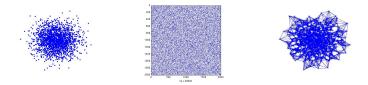
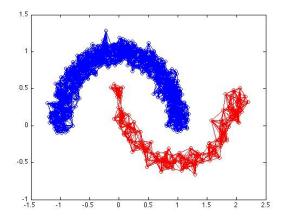


Figure:  $\mu_{degree} = 24.05$ ,  $\sigma_{degree} = 1.41$ 

< < >> < <</p>

# Data Structure to Keep in Mind for Section



 $|C_1| = 2000, |C_2| = 200$ 

Norbert

# **Eigenvalues Determine Order of LE Feature Vectors**

- Order in which LE eigenvectors appear determined by eigenvalue order
- Goal:
  - Characterize eigenvalues of two graph clusters separately
  - Examine interlacing of eigenvalues to determine order of features emerging
- Eigenvalue distribution of k-regular graph is well studied question
  - McKay, 1981 showed empirical spectral distribution of  $\frac{1}{\sqrt{k-1}}A_n$  converges to

$$f_{semi}(x) = \frac{1}{2\pi}\sqrt{4-x^2}, \quad -2 < x < 2$$

Dumitriu, Pal 2013 - found deviation from fsemi for finite graph
 Independently found by Tran, Vu, and Wang 2013

# Eigenvalues Determine Order of LE Feature Vectors

- Order in which LE eigenvectors appear determined by eigenvalue order
- Goal:
  - Characterize eigenvalues of two graph clusters separately
  - Examine interlacing of eigenvalues to determine order of features emerging
- Eigenvalue distribution of k-regular graph is well studied question
  - McKay, 1981 showed empirical spectral distribution of  $\frac{1}{\sqrt{k-1}}A_n$  converges to

$$f_{semi}(x) = rac{1}{2\pi} \sqrt{4 - x^2}, \quad -2 < x < 2$$

イロト イポト イヨト イヨ

- Dumitriu, Pal 2013 found deviation from fsemi for finite graph
- Independently found by Tran, Vu, and Wang 2013

# Eigenvalues of Regular Graph (cont.)

#### Theorem (Dumitriu, Pal, 2012)

Fix  $\delta > 0$  and let  $k = (\log(n))^{\gamma}$ , and let  $\eta = \frac{1}{2}(\exp(k^{-\alpha}) - \exp(-k^{-\alpha}))$ , for  $0 < \alpha < \min(1, 1/\gamma)$ . Then for

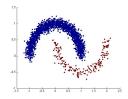
- $G \in \mathcal{G}_{n,k}$  chosen randomly with adjacency matrix A, and
- *interval*  $\mathcal{I} \subset \mathbb{R}$  *such that*  $|\mathcal{I}| \geq \max\{2\eta, \eta/(-\delta \log \delta)\}$ ,

there exists an N large enough such that  $\forall n > N$ ,

$$|\mathcal{N}_{\mathcal{I}} - n \int_{\mathcal{I}} f_{semi}(x) dx| < n \delta |\mathcal{I}|$$

with probability at least 1 - o(1/n). Here,  $\mathcal{N}_l$  is the number of eigenvalues of  $\frac{1}{\sqrt{k-1}}A$  in the interval  $\mathcal{I}$ .

# **Eigenvalues for Disjoint Clusters**



- Consider two clusters  $C_1$  and  $C_2$  with  $|C_1| = D|C_2|$ 
  - $G_1$  and  $G_2$  are generated graphs on  $C_1$  and  $C_2$ , respectively

• 
$$G_1 \in \mathcal{G}_{n,k}$$
 and  $G_2 \in \mathcal{G}_{\frac{n}{D},k}$ 

• 
$$\sigma\left(\frac{1}{\sqrt{k-1}}A_{1}\right)$$
 and  $\sigma\left(\frac{1}{\sqrt{k-1}}A_{2}\right)$  distributed similarly due to Dumitriu and Pal

•  $\sigma(L_1)$  and  $\sigma(L_2)$  distributed similarly on [0, 2]

• Eigenvalues interweave in way that depends on D

#### Eigenvalues for Disjoint Clusters (cont.)

#### Theorem (C., 2014)

Let  $G = (\Omega, E)$  be graph. Suppose  $\Omega$  can be split into two disjoint regular graph clusters  $C_1$  and  $C_2$  such that  $|C_1| = D|C_2| = n$ . Choose any interval  $\mathcal{I} \subset [0, 2]$  such that

$$|\mathcal{I}| \geq \frac{\sqrt{k-1}}{k} \max\{2\eta, \eta/(-\delta \log \delta)\}.$$

Let L denote the graph Laplacian, with eigenpairs  $\{(\sigma_i, v_i)\}_{i=1}^m$  that lie in  $\mathcal{I}$ . Let  $\mathcal{N}_{\mathcal{I}}^1 = |\{i : \operatorname{supp}(v_i) \subset C_1\}|$  and  $\mathcal{N}_{\mathcal{I}}^2 = |\{i : \operatorname{supp}(v_i) \subset C_2\}|$ . Then  $\mathcal{N}_{\mathcal{I}}^1 + \mathcal{N}_{\mathcal{I}}^2 = m$ , and  $\forall n > N$ , with probability at least 1 - o(1/n),

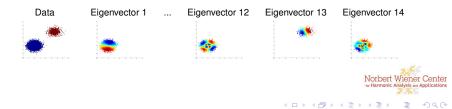
$$|\mathcal{N}_{\mathcal{I}}^{1} - \mathcal{D}\mathcal{N}_{\mathcal{I}}^{2}| \leq 2\delta n \frac{k}{\sqrt{k-1}} |\mathcal{I}|.$$

INOIDEIT VVIENET Center for Harmonic Analysis and Applications

イロト イポト イヨト イヨト

# Eigenvector Localization on Disjoint Graphs

- Theorem implies each eigenvector is localized on either C<sub>1</sub> or C<sub>2</sub>
- Up to error, eigenvector on *C*<sub>2</sub> appears approximately 1 : *D* + 1 times
  - Implies most of energy from LE embedding lies in C<sub>1</sub>
- Applies for any interval  $\mathcal{I} \subset [0,2]$
- Can be generalized to larger number of clusters
- Argument explains initial example shown (D = 10)



#### Sketch of Proof for Disjoint Graphs

• 
$$L = \begin{pmatrix} L_1 & 0 \\ 0 & L_2 \end{pmatrix}$$
  
•  $\sigma(L) = \sigma(L_1) \cup \sigma(L_2)$   
•  $L \begin{pmatrix} v \\ 0 \end{pmatrix} = \lambda \begin{pmatrix} v \\ 0 \end{pmatrix} \iff L_1 v = \lambda v$   
•  $L \begin{pmatrix} 0 \\ v \end{pmatrix} = \lambda \begin{pmatrix} 0 \\ v \end{pmatrix} \iff L_2 v = \lambda v$ 

• Thus all eigenvectors v of L concentrated on one cluster C<sub>i</sub>

- Order determined by  $\sigma(L_1)$  and  $\sigma(L_2)$
- Rescale  $\sigma\left(\frac{1}{\sqrt{k-1}}A\right)$  from Dumitriu and Pal Theorem to  $\sigma(L)$

Because G is k-regular,

$$\frac{1}{\sqrt{k-1}}Av_i = \lambda_i v_i \iff Lv_i = \left(1 - \frac{\sqrt{k-1}}{k}\lambda_i\right)v_i$$
Norbert Wiener Center  
we Harmonic Analysis as Applications

#### Sketch of Proof for Disjoint Graphs

• 
$$L = \begin{pmatrix} L_1 & 0 \\ 0 & L_2 \end{pmatrix}$$
  
•  $\sigma(L) = \sigma(L_1) \cup \sigma(L_2)$   
•  $L \begin{pmatrix} v \\ 0 \end{pmatrix} = \lambda \begin{pmatrix} v \\ 0 \end{pmatrix} \iff L_1 v = \lambda v$   
•  $L \begin{pmatrix} 0 \\ v \end{pmatrix} = \lambda \begin{pmatrix} 0 \\ v \end{pmatrix} \iff L_2 v = \lambda v$ 

• Thus all eigenvectors v of L concentrated on one cluster C<sub>i</sub>

- Order determined by  $\sigma(L_1)$  and  $\sigma(L_2)$
- Rescale  $\sigma\left(\frac{1}{\sqrt{k-1}}A\right)$  from Dumitriu and Pal Theorem to  $\sigma(L)$

• Because G is k-regular,

$$\frac{1}{\sqrt{k-1}}Av_i = \lambda_i v_i \iff Lv_i = (1 - \frac{\sqrt{k-1}}{k}\lambda_i)v_i$$
Norbert Wiener Center
te Harmonic Analysis of Applications

# Sketch of Proof (cont.)

• Design parameters from Dumitriu and Pal Theorem that are constant across both clusters *C<sub>i</sub>* 

• Interval  $\mathcal{I}$  for  $\sigma(L)$  has corresponding interval  $\mathcal{I}_A$  for  $\sigma(\frac{1}{\sqrt{k-1}}A)$ 

Theorem guarantees that

$$|\mathcal{N}_{\mathcal{I}_A}^1 - n \int_{\mathcal{I}_A} f_d(x) dx| < n\delta |\mathcal{I}_A|,$$
  
 $|\mathcal{N}_{\mathcal{I}_A}^2 - rac{n}{D} \int_{\mathcal{I}_A} f_d(x) dx| < rac{n}{D} \delta |\mathcal{I}_A|.$ 

This means

$$\begin{split} |\mathcal{N}_{\mathcal{I}}^{1} - \mathcal{D}\mathcal{N}_{\mathcal{I}}^{2}| &\leq |\mathcal{N}_{\mathcal{I}_{A}}^{1} - n \int_{\mathcal{I}_{A}} f_{d}(x) dx| + |\mathcal{D}\mathcal{N}_{\mathcal{I}_{A}}^{2} - n \int_{\mathcal{I}_{A}} f_{d}(x) dx| \\ &\leq 2n\delta |\mathcal{I}_{A}| \\ &= 2n\delta \frac{k}{\sqrt{k-1}} |\mathcal{I}| \end{split}$$
 Nothert Wiener Centre of the Harmonic Analysis as Application of the Harmonic Analysis and the Harmonic Analysis as Application of the Harmonic Analysis as App

## Sketch of Proof (cont.)

• Design parameters from Dumitriu and Pal Theorem that are constant across both clusters *C<sub>i</sub>* 

• Interval  $\mathcal{I}$  for  $\sigma(L)$  has corresponding interval  $\mathcal{I}_A$  for  $\sigma(\frac{1}{\sqrt{k-1}}A)$ 

Theorem guarantees that

$$|\mathcal{N}_{\mathcal{I}_{A}}^{1} - n \int_{\mathcal{I}_{A}} f_{d}(x) dx| < n\delta |\mathcal{I}_{A}|,$$
  
 $|\mathcal{N}_{\mathcal{I}_{A}}^{2} - rac{n}{D} \int_{\mathcal{I}_{A}} f_{d}(x) dx| < rac{n}{D} \delta |\mathcal{I}_{A}|.$ 

This means

$$\begin{split} |\mathcal{N}_{\mathcal{I}}^{1} - \mathcal{D}\mathcal{N}_{\mathcal{I}}^{2}| &\leq |\mathcal{N}_{\mathcal{I}_{A}}^{1} - n \int_{\mathcal{I}_{A}} f_{d}(x) dx| + |\mathcal{D}\mathcal{N}_{\mathcal{I}_{A}}^{2} - n \int_{\mathcal{I}_{A}} f_{d}(x) dx| \\ &\leq 2n\delta |\mathcal{I}_{A}| \\ &= 2n\delta \frac{k}{\sqrt{k-1}} |\mathcal{I}| \end{split}$$

### **Disjoint Graph Conclusions**

#### Important notes from Theorem

- Characterizes order of feature vectors from LE
- Demonstrates that, among first *m* eigenvectors,  $\frac{D}{D+1}$  of them are concentrated in largest cluster
- Attempt to design LE similarity kernel such that graph as disjoint as possible
- Arguments generalize to larger number of clusters

#### Drawbacks

- In practice, cannot design disconnected graph from data
- Need to add edges to connect graph for better theory
- Already know Fiedler vector is highly sensitive to connecting edge

< □ > < 同 > < 回 > <

## **Disjoint Graph Conclusions**

#### Important notes from Theorem

- Characterizes order of feature vectors from LE
- Demonstrates that, among first *m* eigenvectors,  $\frac{D}{D+1}$  of them are concentrated in largest cluster
- Attempt to design LE similarity kernel such that graph as disjoint as possible
- Arguments generalize to larger number of clusters
- Drawbacks
  - In practice, cannot design disconnected graph from data
  - Need to add edges to connect graph for better theory
  - Already know Fiedler vector is highly sensitive to connecting edge

< □ > < □ > < □ > < □ >

#### Outline



2 Characterizing Embeddings for Disjoint Graphs

#### Eigenvector Localization of Graphs with Weakly Connected Clusters





#### Weakly Connected Clusters

#### Definition

A graph with *weakly connected clusters of order t* is a connected graph with adjacency matrix

$$A = egin{pmatrix} A_1 & B_{1,2} \ B_{1,2}^\intercal & A_2 \end{pmatrix},$$

where

A1 and A2 are adjacency matrices of k-regular graphs, and

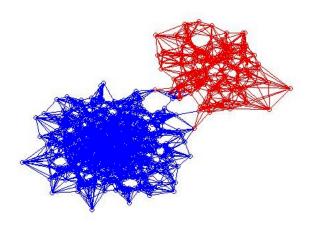
2  $B_{1,2}$  has t non-zero entries.

We shall refer to the nodes of  $A_1$  as  $C_1$  and the nodes of  $A_2$  as  $C_2$ 

Norbert Wiener Center

(日)

#### Weakly Connected Clusters Example





# Weakly Connected Clusters as Matrix Perturbation

- Now problem is characterized by perturbation of known matrix
  - *G* is weakly connected graph with adjacency  $A = \begin{pmatrix} A_1 & B_{1,2} \\ B_1^T & A_2 \end{pmatrix}$
  - *H* is disjoint graph with adjacency  $A = \begin{pmatrix} A_1 & 0 \\ 0 & A_2 \end{pmatrix}$
- Let  $L_G$  be normalized Laplacian of G, and similar for  $L_H$

#### Perturbation of $L_{H}$

 $L_G = L_H + E$ , where  $||E||_F \ll ||L_H||_F$ 

#### Questions:



Is eigenvalue ordering of L<sub>G</sub> drastically affected?

Are eigenvectors of L<sub>G</sub> still concentrated on clusters?



### **Eigenvalue Distribution for GWCC**

#### Theorem (Chen, et. al., 2012)

Let  $G = (\Omega, E_G)$  and  $H = (\Omega, E_H)$  be spanning graphs such that  $|E(G - H)| \le t$ . If

 $\lambda_1 \leq \ldots \leq \lambda_n$ , and  $\theta_1 \leq \ldots \leq \theta_n$ 

are the eigenvalues of the normalized Laplacians  $L_G$  and  $L_H$  respectively, then

$$\theta_{i-t} \leq \lambda_i \leq \theta_{i+t}, \qquad 1 \leq i \leq n,$$

with the convention that  $\theta_{-t} = ... = \theta_0 = 0$  and  $\theta_{n+1} = ... = \theta_{n+t} = 2$ .

- Related to Weyl's inequality and Courant-Fischer theorem
- Shows why lowest eigenvalues difficult to predict
- Will lead to issues with Fiedler vector

# Eigenvalue Distribution for GWCC (cont.)

#### Lemma (C., 2014)

Let  $G = (\Omega, E)$  be a graph with weakly connected clusters of order *t*, with

•  $|C_1| = n$ ,

• 
$$|C_2| = \frac{n}{D}$$
.

Fix  $\delta$ , k,  $\alpha$ ,  $\eta$ , and  $\mathcal{I}$  as in Theorem for disjoint clusters. Let L denote the graph Laplacian, and  $\sigma_1, ..., \sigma_m$  denote the m eigenvalues of L that lie in  $\mathcal{I}$ . Then m satisfies

$$|m-(n+rac{n}{D})\int_{\mathcal{I}}f_{semi}(x)dx| < \delta(n+rac{n}{D})rac{k}{\sqrt{k-1}}|\mathcal{I}|+2t,$$
 (1)

again with probability at least 1 - o(1/n).

## Invariant Subspace Perturbations

- Eigenvectors under perturbation require more careful treatment
- Dependent on separation of spectrum

# Example Let $A = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \implies \sigma(A) = \{1\}, \ V = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}.$ Let $\widetilde{A} = \begin{pmatrix} 1 & \epsilon \\ \epsilon & 1 \end{pmatrix} \implies \sigma(\widetilde{A}) = \{1 - \epsilon, 1 + \epsilon\}, \ \widetilde{V} = \begin{pmatrix} 1 & -1 \\ 1 & 1 \end{pmatrix}.$

- Introduced by Davis 1963 for single eigenvector
- Generalized by Davis and Kahan 1970
- "Matrix Perturbation Theory" by Stewart and Sun 1990
- Localization of QR, LU, and Cholesky by Krishtal, Strohmer, and Wertz

イロト イポト イヨト イヨト

• Studied on graphs by Rajapakse 2013

### Invariant Subspace Perturbations (cont.)

#### Theorem (Davis, 1963)

Let  $A, E \in \mathbb{C}^{n \times n}$ . Let  $(\lambda, x)$  be an eigenpair of A such that

$$\operatorname{sep}(\lambda, \sigma(A) \setminus \lambda) = \min\{|\lambda - \gamma| : \gamma \in \sigma(A) \setminus \lambda\} = \delta.$$

Let

- P be a spectral projector of A such that Px = x
- P' be the corresponding spectral projector of A + E, and
- $\overline{P'}z = z P'z$ .

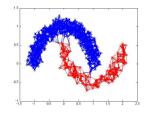
Then if  $||E|| \le \epsilon \le \delta/2$ ,

$$\|\overline{P'}P\| \leq \frac{\epsilon}{\delta - \epsilon}.$$

for Harmonic Analysis and Application

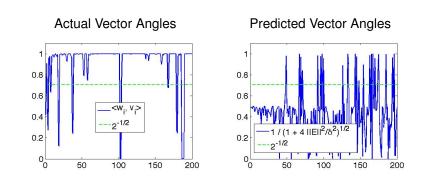
# Poor Prediction Using Existing Theory

- Consider two moons example
  - {(\$\tilde{\lambda}\_i, \mathbf{v}\_i\$)} eigenpairs of weakly connected graph \$L\_G\$
  - $\{(\lambda_i, w_i)\}$  eigenpairs of disjoint graph  $L_H$
  - Generate L<sub>H</sub> by removing off block diagonal entries



- $\sigma(L_H) \in [0, 2]$  is not sufficiently separated for existing theory
- Assumptions in literature are too strict for problem
- Also we are interested in localization, not angle

# Poor Prediction Using Existing Theory (cont.)



Norbert Wie

A B A B A
 A
 B
 A
 A
 B
 A
 A
 B
 A
 A
 B
 A
 A
 B
 A
 A
 B
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A
 A

## Eigengap Dependence on Similar Eigenvectors

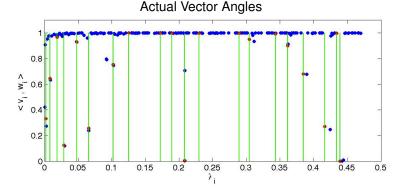
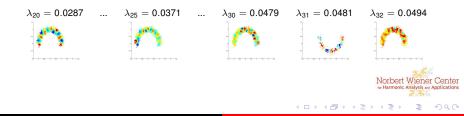


Figure: Green Line Denotes Eigenvector of L<sub>H</sub> Concentrated on Smaller C<sub>2</sub> Cluster

Norbert Wiener Center

# Eigengap Dependence on Similar Eigenvectors (cont.)

- Problem eigenvector w<sub>i</sub> follows pattern
  - $supp(w_i) \subset C_2$
  - $supp(w_{i-1}) \subset C_1$
  - $supp(w_{i+1}) \subset C_1$
- This is case for most eigenvectors from smaller C<sub>2</sub> cluster
  - $|C_1| = D|C_2| \implies \frac{D}{D+1}$  eigenvectors of  $L_H$  concentrated on  $C_1$
- Consider eigenvector w<sub>25</sub> of L<sub>H</sub> as example



## **Eigenvector Localization**

#### Theorem (C., 2014)

Let  $L_H \in \mathbb{R}^{n \times n}$  be symmetric with eigendecomposition  $L_H = V \Sigma V^*$ . Let  $(\lambda_i, v_i)$  be an eigenpair of  $L_H$ . Partition  $V = [V_1, V_2, v_i, V_3, V_4]$  where  $V_2, V_3 \in \mathbb{R}^{n \times s}$ . Moreover, assume  $\exists C \subsetneq \{1, ..., n\}$  such that  $supp(v_i) \subset C$  and  $supp(v_j) \subset C$  where  $v_j$  is a column of  $V_2, V_3$ . Let  $(\widetilde{\lambda}, x)$  an eigenvector of the perturbed matrix  $L_G = L_H + E$ , where  $x = [x_1, ..., x_n]$ . Then

$$\sum_{j\in C^c} |x_j|^2 \leq \frac{\|(\widetilde{\lambda}-\lambda_i)x-Ex\|_2^2}{\min(\lambda_i-\lambda_{i-s},\lambda_{i+s}-\lambda_i)^2}.$$

- Apply SVD Theorem to symmetric matrix  $L_H \lambda_i I$ 
  - SVD equivalence with eigendecomposition up to parity



Singular Vector Localization

#### Theorem (C., 2014)

Let  $A \in \mathbb{R}^{n \times n}$  with SVD  $A = U \Sigma V^*$ . Partition

 $V=[V_1, V_2, v_n],$ 

where  $v_n \in \mathbb{R}^n$ ,  $V_2 \in \mathbb{R}^{n \times s}$ . Moreover, assume  $\exists C \subsetneq \{1, ..., n\}$  such that

 $\operatorname{supp}(v_i) \subset C \quad \text{for} \quad i \in \{n-s, ..., n\}.$ 

Let  $x \in \mathbb{R}^n$  such that  $||x||_2 = 1$ . Then

$$\sum_{i \in C^c} |x_i|^2 \leq \frac{\|Ax\|_2^2 - \|Av_n\|_2^2}{\sigma_{n-s-1}^2(A) - \sigma_n^2(A)}.$$

Center

イロト イポト イヨト イヨト

### Sketch of Proof for SVD Localization

Assume  $x = V_1 c_1 + V_2 c_2 + v_n c_3$ . Bound

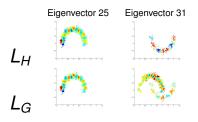
$$\begin{aligned} \|Ax\|_{2}^{2} &= \|U_{1}\Sigma_{1}V_{1}^{*}x + U_{2}\Sigma_{1}V_{2}^{*}x + u_{n}\sigma_{n}v_{n}^{*}x\|_{2}^{2} \\ &\implies \|Ax\|_{2}^{2} - \|Av_{n}\|_{2}^{2} \geq (\sigma_{n-s-1}^{2} - \sigma_{n}^{2})\|c_{1}\|_{2}^{2} \\ &\implies \|c_{1}\|_{2}^{2} \leq \frac{\|Ax\|_{2}^{2} - \|Av_{n}\|_{2}^{2}}{\sigma_{n-s-1}^{2} - \sigma_{n}^{2}}. \end{aligned}$$

Using the localization of  $V_2$ ,

$$\sum_{i \in C^{c}} |x_{i}|^{2} \leq \sum_{i=1}^{n} \sum_{j=1}^{n-s-1} |(V_{1})_{i,j}c_{j}|^{2}$$
$$= \sum_{j=1}^{n-s-1} |c_{j}|^{2}$$
$$\leq \frac{||Ax||_{2}^{2} - ||Av_{n}||_{2}^{2}}{\sigma_{n-s-1}^{2} - \sigma_{n}^{2}}.$$

Norbert Wiener Center w Harmonic Analysis w Applications

## **Eigenvector Localization Conclusions**



- Important notes from Theorem
  - Theorem implies 124 of 180 eigenvectors supported on *C*<sub>1</sub> remain concentrated

• • • • • • • • • • • •

- Only 3 of 20 eigenvectors supported on C<sub>2</sub> remain concentrated
- Makes determining inter-cluster differences difficult for small clusters

### Outline



2 Characterizing Embeddings for Disjoint Graphs

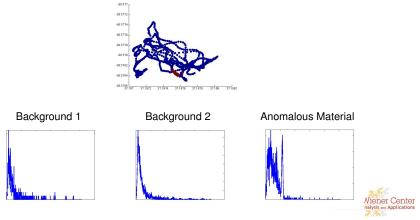
3 Eigenvector Localization of Graphs with Weakly Connected Clusters





## Nuclear Data

- Wish to detect anomalous material that emit radiation
- Build LE graph from radiological spectra

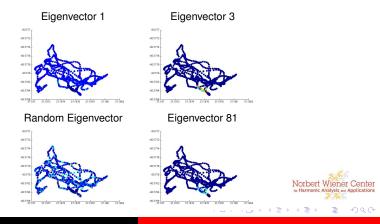


• • • • • • • • • • • • •

Data courtesy of Kevin Kochersberger, Virginia Tech

# Anomalous Clusters Washed Out

- Use simple L<sup>2</sup> distance to create binary similarity kernel, 10 nearest neighbors
- # background measurements = 1137, # anomalous measurements = 23
  - $D = 49.4 \implies$  energy on anomalous cluster shows up 1 : 50 times at best
  - All other eigenvectors (not shown) are only noise



# Conclusions

- Takeaways:
  - Small clusters in disjoint graphs appear rarely in LE feature vectors
    - Proportional to number of data points in cluster
  - LE eigenvectors concentrated on small cluster rarely remain localized as graph becomes connected
  - Eigenvectors concentrated on larger cluster almost always remain localized
    - Leads to points on small cluster being forced to zero
  - Phenomenon is supported by simulated and real-world data

#### • Future Directions:

- Upper bound on localization theory that doesn't require A + E eigenvector
- Theory for anomalous clusters that are smaller than k data points
- Alter selection to subset of "low-frequency" eigenfunctions
  - Subset of indices originally introduced by Jones, Maggioni, Schul Notbert Wiener Cen 2010

< □ > < 同 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < 回 > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □ > < □

# Conclusions

- Takeaways:
  - Small clusters in disjoint graphs appear rarely in LE feature vectors
    - Proportional to number of data points in cluster
  - LE eigenvectors concentrated on small cluster rarely remain localized as graph becomes connected
  - Eigenvectors concentrated on larger cluster almost always remain localized
    - · Leads to points on small cluster being forced to zero
  - Phenomenon is supported by simulated and real-world data
- Future Directions:
  - Upper bound on localization theory that doesn't require *A* + *E* eigenvector
  - Theory for anomalous clusters that are smaller than k data points
  - Alter selection to subset of "low-frequency" eigenfunctions
    - Subset of indices originally introduced by Jones, Maggioni, Schul 2010

< □ > < 同 > < 回 > <

# Thank you!



# **Extra Slides**



# **Eigenvalues of Regular Graph**

#### Theorem (McKay, 1981)

Let  $X_1, X_2, ...$  be a sequence of random k-regular graphs with adjacency matrices  $A_1, A_2, ...$ 

Let the family  $\{X_i\}$  satisfy

$$In(X_i) \to \infty$$

$$c_k(X_i)/n(X_i) \to 0.$$

Then the empirical spectral distribution

$$F_n(x) = |\{i : \lambda_i \left(\frac{1}{\sqrt{k-1}}A_n\right) < x\}|/n$$

converges pointwise to the semicircle law

$$f_{semi}(x) = rac{1}{2\pi} \sqrt{4-x^2}, \quad -2 < x < 2.$$

Center plications

< ロ > < 同 > < 回 > < 回 >

## Invariant Subspace Perturbations (cont.)

#### Theorem (Davis, 1963)

Let  $A, E \in \mathbb{C}^{n \times n}$ . Let  $(\lambda, x)$  be an eigenpair of A such that

$$\operatorname{sep}(\lambda, \sigma(A) \setminus \lambda) = \min\{|\lambda - \gamma| : \gamma \in \sigma(A) \setminus \lambda\} = \delta.$$

Let

- P be a spectral projector of A such that Px = x
- P' be the corresponding spectral projector of A + E, and
- $\overline{P'}z = z P'z$ .

Then if  $\|E\| \le \epsilon \le \delta/2$ ,

$$\|\overline{P'}P\| \leq \frac{\epsilon}{\delta - \epsilon}.$$

for Harmonic Analysis and Application

## Invariant Subspace Perturbations (cont.)

#### Theorem (Stewart, 1973)

Let  $A, E \in \mathbb{C}^{n \times n}$ . Let  $X = [X_1, X_2]$  be a unitary matrix with  $X_1 \in \mathbb{C}^{n \times l}$ , and suppose  $\mathcal{R}(X_1)$  is an invariant subspace of A. Let

$$X^*AX = \begin{pmatrix} A_{1,1} & A_{1,2} \\ 0 & A_{2,2} \end{pmatrix}, \quad X^*EX = \begin{pmatrix} E_{1,1} & E_{1,2} \\ E_{2,1} & E_{2,2} \end{pmatrix}$$

Let  $\delta = sep(A_{1,1}, A_{2,2}) - ||E_{1,1}|| - ||E_{2,2}||$ . Then if

$$\frac{\|E_{2,1}\|(\|A_{1,2}\|+\|E_{1,2}\|)}{\delta^2} \leq \frac{1}{4},$$

there is a matrix P satisfying  $\|P\| \le 2\frac{\|E_{2,1}\|}{\delta}$  such that

$$\widetilde{X_1} = (X_1 + X_2 P)(I + P^* P)^{-1/2}$$

is an invariant subspace of A + E.

