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National Institute of Informatics

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Semi-Supervised Graph Classifier Learning with Negative Edge Weights

Acknowledgement

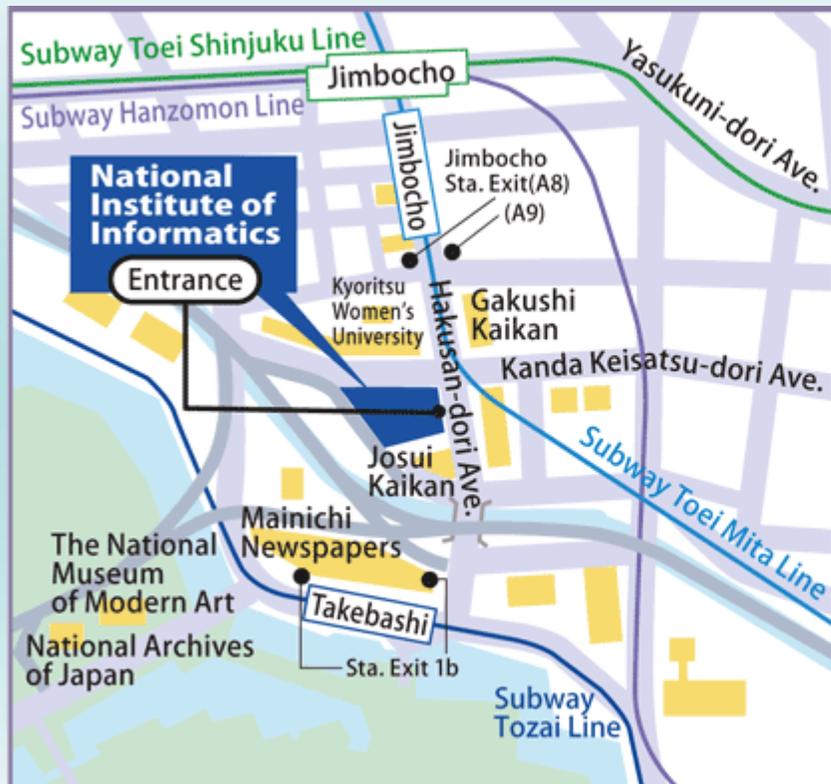
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NII Overview

- **National Institute of Informatics**
- Chiyoda-ku, Tokyo, Japan.
- Government-funded research lab.
- Offers graduate courses & degrees through **The Graduate University for Advanced Studies** (Sokendai).
- 60+ faculty in “**informatics**”: quantum computing, discrete algorithms, database, machine learning, computer vision, speech & audio, image & video processing.



- **Get involved!**
 - 2-6 month Internships.
 - Short-term visits via MOU grant.
 - Lecture series, Sabbatical.

Introduction to APSIPA and APSIPA DL

APSIPA Mission: To promote broad spectrum of research and education activities in signal and information processing in Asia Pacific

APSIPA Conferences: ASIIPA Annual Summit and Conference

APSIPA Publications: Transactions on Signal and Information Processing in partnership with Cambridge Journals since 2012; APSIPA Newsletters

APSIPA Social Network: To link members together and to disseminate valuable information more effectively

APSIPA Distinguished Lectures: An APSIPA educational initiative to reach out to the community



Outline

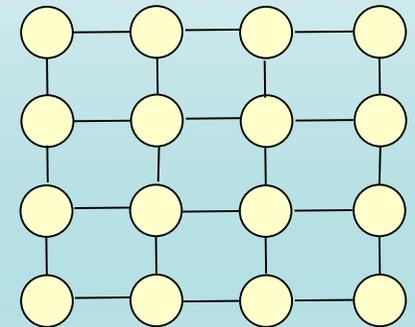
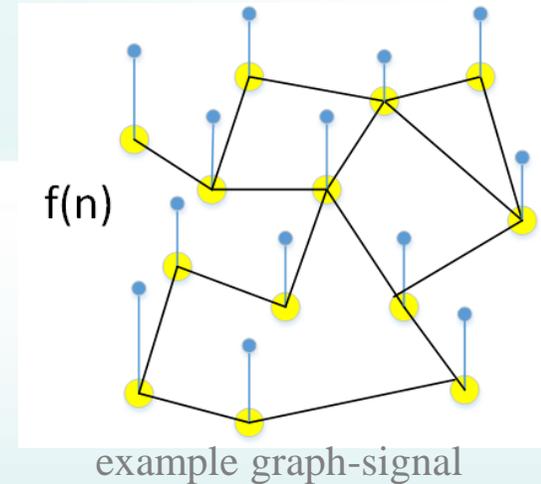
- Graph Signal Processing
 - Graph spectrum
- Semi-supervised Graph Classifier
 - Smoothness prior & MAP formulation
 - Graph construction
 - Graph Laplacian perturbation
 - Lower bound min eigenvalue computation
 - IRLS algorithm
- Experimental Results
- Conclusion

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Graph Signal Processing

- Signals on **irregular** data kernels described by graphs.
 - Graph: nodes and edges.
 - Edges reveals *node-to-node relationships*.
1. Data domain is naturally a graph.
 - **Ex:** ages of users on social networks.
 2. Underlying data structure unknown.
 - **Ex:** images: 2D grid \rightarrow structured graph.

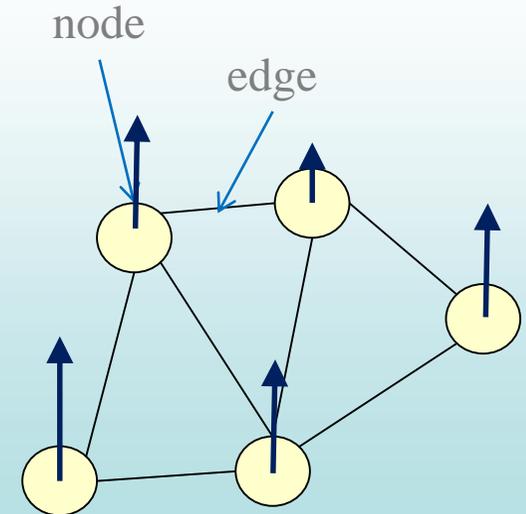


Graph Signal Processing (GSP) addresses the problem of processing signals that live on graphs.

Graph Signal Processing

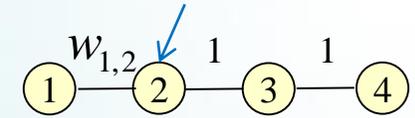
Research questions*:

- **Sampling**: how to efficiently acquire / sense a graph-signal?
 - Graph sampling theorems.
- **Representation**: Given graph-signal, how to compactly represent it?
 - Transforms, wavelets, dictionaries.
- **Signal restoration**: Given noisy and/or partial graph-signal, how to recover it?
 - Graph-signal priors.



Graph Fourier Transform (GFT)

undirected graph



$$A = \begin{bmatrix} 0 & w_{1,2} & 0 & 0 \\ w_{1,2} & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$D = \begin{bmatrix} w_{1,2} & 0 & 0 & 0 \\ 0 & w_{1,2} + 1 & 0 & 0 \\ 0 & 0 & 2 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$L = \begin{bmatrix} w_{1,2} & -w_{1,2} & 0 & 0 \\ -w_{1,2} & w_{1,2} + 1 & -1 & 0 \\ 0 & -1 & 2 & -1 \\ 0 & 0 & -1 & 1 \end{bmatrix}$$

Graph Laplacian:

- **Adjacency Matrix A:** entry $A_{i,j}$ has *non-negative* edge weight $w_{i,j}$ connecting nodes i and j .
- **Degree Matrix D:** diagonal matrix w/ entry $D_{i,i}$ being sum of column entries in row i of A .

$$D_{i,i} = \sum_j A_{i,j}$$

- **Combinatorial Graph Laplacian L:** $L = D - A$

- L is *symmetric* (graph undirected).
- L is a *high-pass* filter.
- L is related to *2nd derivative*.

$$L_{3,:} x = -x_2 + 2x_3 - x_4$$

$$f''(x) = \lim_{h \rightarrow 0} \frac{f(x+h) - 2f(x) + f(x-h)}{h^2}$$

Graph Spectrum from GFT

- **Graph Fourier Transform** (GFT) is eigen-matrix of graph Laplacian L .

$$L u_i = \lambda_i u_i$$

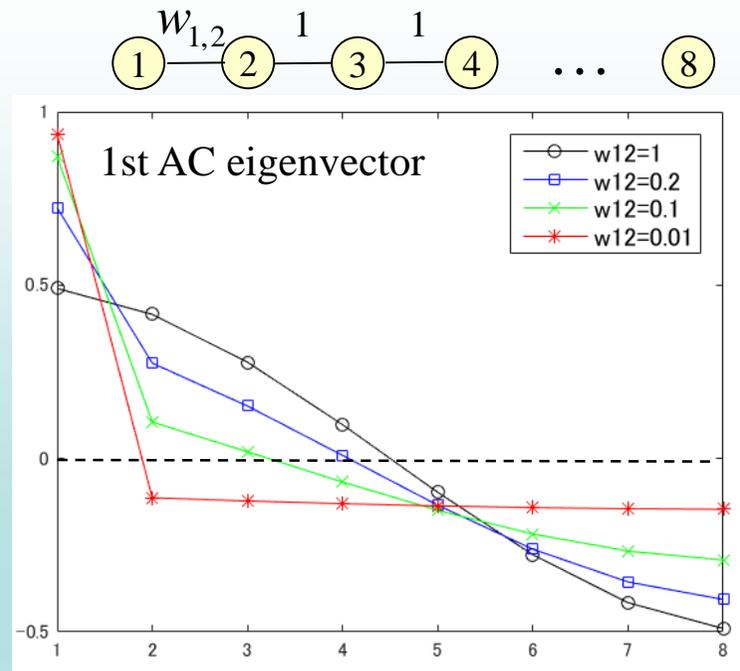
← eigenvalue
← eigenvector

1. Edge weights affect shapes of eigenvectors.

2. Eigenvalues (≥ 0) as *graph frequencies*.

- Constant eigenvector is DC.
- # *zero-crossings* increases as λ increases.

- GFT defaults to **DCT** for un-weighted connected line.
- GFT defaults to **DFT** for un-weighted connected circle.



Variants of Graph Laplacians

- **Graph Fourier Transform** (GFT) is eigen-matrix of graph Laplacian L .

$$L u_i = \lambda_i u_i$$

← eigenvalue ← eigenvector

- Other definitions of graph Laplacians:

- **Normalized** graph Laplacian:

$$L_n = D^{-1/2} L D^{-1/2} = I - D^{-1/2} A D^{-1/2}$$

- **Random walk** graph Laplacian:

$$L_{rw} = D^{-1} L = I - D^{-1} A$$

- **Generalized** graph Laplacian [1]:

$$L_g = L + D^*$$

Characteristics:

- Normalized.
- Symmetric.
- No DC component.

- Normalized.
- Asymmetric.
- Eigenvectors not orthog.

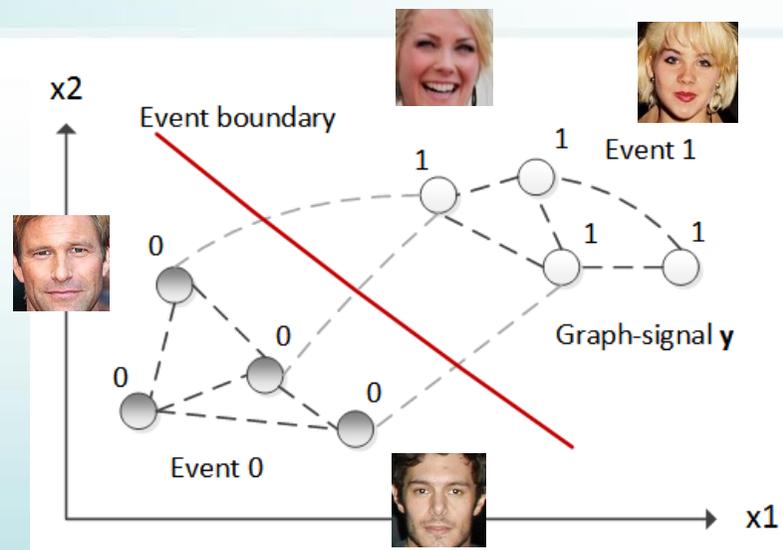
- Symmetric.
- L plus self loops.
- Defaults to DST, ADST.

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Semi-Supervised Graph Classifier Learning

- **Binary Classifier:** given feature vector x_i of dimension K , compute $f(x_i) \in \{0,1\}$.
- **Classifier Learning:** given partial / noisy labels (x_i, y_i) , train classifier $f(x_i)$.



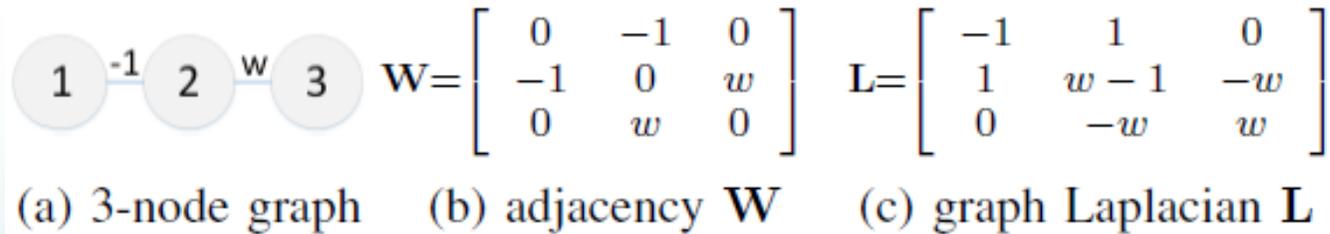
example graph-based classifier

- **GSP Approach [1]:**
 1. Construct **similarity graph** with +/- edges.
 2. Pose MAP graph-signal restoration problem.
 3. Perturb graph Laplacian to ensure PSD.
 4. Solve num. stable MAP as sparse lin. system.

[1] Yu Mao, Gene Cheung, Chia-Wen Lin, Yusheng Ji, "Image Classifier Learning from Noisy Labels via Generalized Graph Smoothness Priors," *IEEE IVMSWP Workshop*, Bordeaux, France, July 2016. (**Best student paper award**)

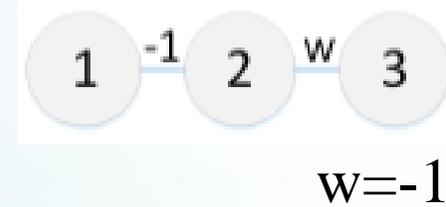
[2] G. Cheung, W.-T. Su, Y. Mao, C.-W. Lin, "Robust Semi-Supervised Graph Classifier Learning with Negative Edge Weights," submitted to Special Issue on "Graph Signal Processing" in *IEEE Journal on Selected Topics of Signal Processing*, November 2016. (arXiv)

Graph-Signal Smoothness Prior



- **Smoothness:** signal “consistent” w/ underlying graph.
- **Q1:** how to define smoothness w.r.t. graph with +/- edges?
- **Q2:** is signal smoothness prior robust to errs?
- **Q3:** is signal smoothness prior easy to solve?

Graph-Signal Smoothness Prior: Candidate 1



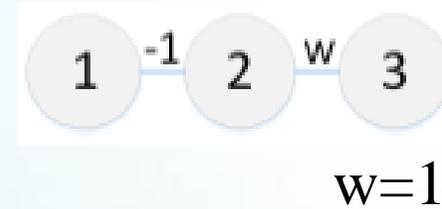
- **Shift-based Smoothness Prior [1]:**

$$\begin{aligned}\|x - \mathbf{W}x\|_2^2 &= \|(\mathbf{I} - \mathbf{W})x\|_2^2 = \left\| \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \right\|_2^2 \\ &= (x_1 + x_2)^2 + (x_1 + x_2 + x_3)^2 + (x_2 + x_3)^2\end{aligned}$$

shifted version of signal

- Prior minimizes sums of sample values despite negative edges!

Graph-Signal Smoothness Prior: Candidate 2



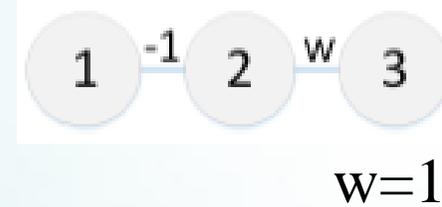
- **Total Variation (TV) [1] on graph:**

$$|\mathbf{Lx}| = \left| \begin{bmatrix} -1 & 1 & 0 \\ 1 & 0 & -1 \\ 0 & -1 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \right| = \begin{bmatrix} x_2 - x_1 \\ x_1 - x_3 \\ x_3 - x_2 \end{bmatrix}$$

degree 0 at node 2

- Prior minimizes diffs in every pair!

Graph-Signal Smoothness Prior: Candidate 3



- **Graph Laplacian Regularizer [1]:**

$$\mathbf{x}^T \mathbf{L} \mathbf{x} = \sum_{(i,j) \in \mathcal{E}} w_{i,j} (x_i - x_j)^2 = \sum_k \lambda_k \alpha_k^2$$

GFT coeff

eigenvalues / graph freqs

- Promote large / small inter-node differences depending on edge signs.

$$\mathbf{x}^T \mathbf{L} \mathbf{x} = -1(x_1 - x_2)^2 + (x_2 - x_3)^2$$

Promote large difference

Promote small difference

- Sensible, but numerically unstable.

MAP Problem Formulation

- **Label Noise Model:** uniform noise model [1]

$$Pr(y_i|x_i) = \begin{cases} 1 - p & \text{if } y_i = x_i \\ p & \text{o.w.} \end{cases}$$

- Probability of observing noisy \mathbf{y} given ground truth \mathbf{x} :

$$Pr(\mathbf{y}|\mathbf{x}) = p^k (1 - p)^{K-k}$$
$$k = \|\mathbf{y} - \mathbf{H}\mathbf{x}\|_0$$

- MAP formulation:

$$\min_{\mathbf{x}} \|\mathbf{y} - \mathbf{H}\mathbf{x}\|_0 + \mu \mathbf{x}^T (\mathbf{L} + \Delta) \mathbf{x}$$

fidelity term

*perturbation matrix
to ensure PSD!*

graph-signal
smoothness prior

Graph Construction: add positive edges

- Given feature vector per sample in high dim. space.
- First to construct (dis)similarity graph with +/- edges from features.
- Positive edge weights reflect inter-node **similarity**:

$$w_{i,j} = \exp \left(-\frac{(\mathbf{h}_i - \mathbf{h}_j)^T \Xi (\mathbf{h}_i - \mathbf{h}_j)}{\sigma_h^2} \right)$$

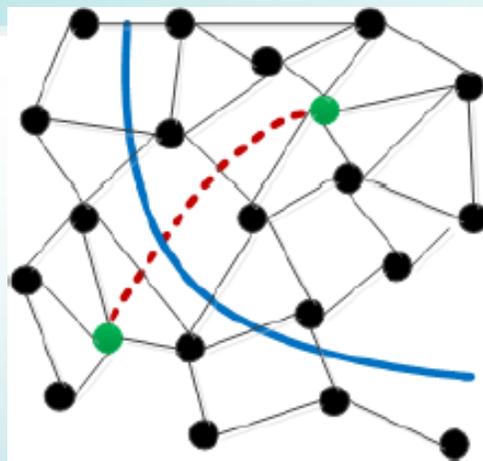
inter-node
feature distance

- Optimization of feature weights in [1].

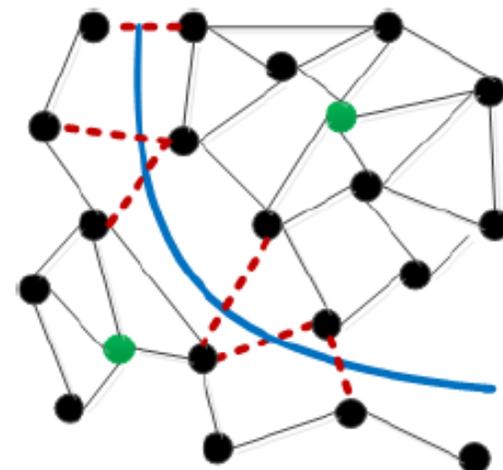
Graph Construction: add negative edges

Centroid-based: add negative edge connecting cluster centroids.

- Robust, not precise.



a) centroid-based graph



b) boundary-based graph

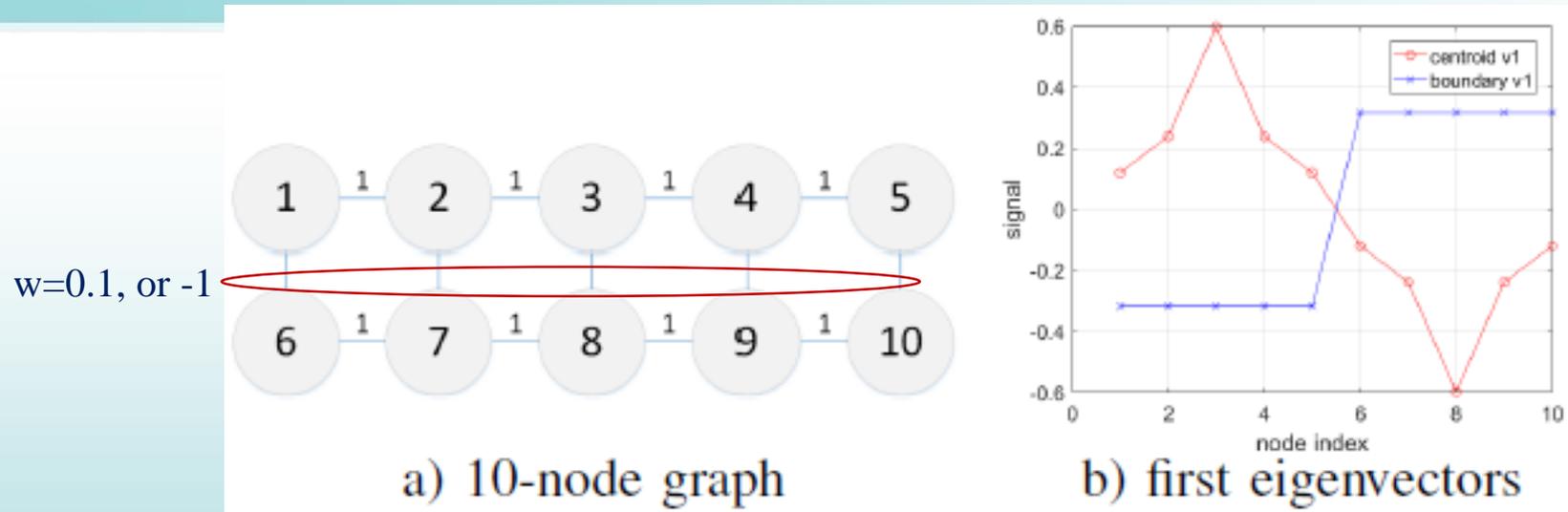
Boundary-based: add negative edges connecting boundary nodes of two clusters.

- Precise, not robust.

Idea: use convex combination as we iterate:

$$\mathbf{L}^* = \beta(\mathbf{L}^1 + \Delta^1) + (1 - \beta)(\mathbf{L}^2 + \Delta^2)$$

Example: 10-node graph



- **Centroid-based 1st e-vector:** peaks at neg. edge endpoints.
- **Boundary-based 1st e-vector:** same level @ boundary nodes.
- Low graph frequencies of indefinite L are useful in restoration [1].

Finding Perturbation Matrix: min norm

- **Minimum norm criteria:** smallest Δ to ensure PSD:

$$\min_{\Delta} \|\Delta\| \quad \text{s.t.} \quad \mathbf{x}^T (\mathbf{L} + \Delta) \mathbf{x} \geq 0, \quad \forall \mathbf{x}$$

$$\mathbf{L} = \mathbf{V} \Lambda \mathbf{V}^T$$

assume has p negative eigenvalues

- Sol'n is special case of Thm 5.1 in [1]:

$$\Delta = \mathbf{V} \text{diag}(\tau) \mathbf{V}^T$$

$$\tau_i = \begin{cases} -\lambda_i & \text{if } 1 \leq i \leq p \\ 0 & \text{o.w.} \end{cases}$$

- **Observations:**

1. $\mathbf{L} + \Delta$ is PSD (good).
2. $\mathbf{L} + \Delta$ preserves same eigen-vectors (good).
3. Eigenvalue 0 has $p+1$ eigen-vectors (bad).

Finding Perturbation Matrix: eigen-structure preservation

- Perturb to ensure PSD while preserving *frequency components* (eigenvectors) and *frequency preferences*.
- One sol'n is $\Delta = \lambda_{\min} I$, i.e. shift all eigenvalues up by $\eta = \lambda_{\min}$.
- **Intuition:** signal variations + signal energies

$$\mathbf{x}^T (\mathbf{L} + \Delta) \mathbf{x} = \mathbf{x}^T \mathbf{L} \mathbf{x} + \eta \mathbf{x}^T \mathbf{I} \mathbf{x}$$

$$= \sum_{i,j} w_{i,j} (x_i - x_j)^2 + \eta \sum_i x_i^2$$

signal variations

signal energies

- **Q:** computed lower-bound for λ_{\min} w/o eigen-decomposition?

Lower Bound λ_{\min}

- Matrix Inertia:

$$\text{In}(\mathbf{A}) = (i^+(\mathbf{A}), i^-(\mathbf{A}), i^0(\mathbf{A}))$$

- Haysworth Inertia Additivity:

$$\text{In}(\mathbf{L}) = \text{In}(\mathbf{L}_{1,1}) + \text{In}(\mathbf{L}/\mathbf{L}_{1,1})$$

Schur complement

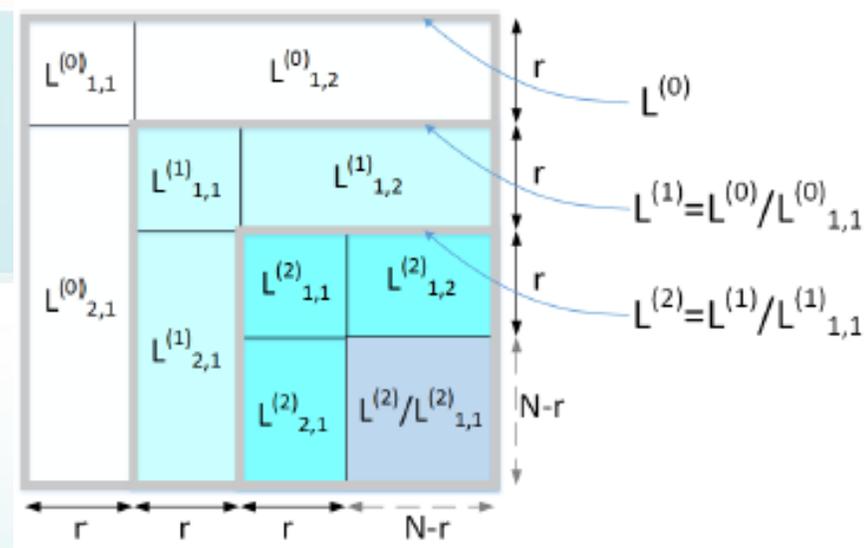
$$\mathbf{L}/\mathbf{L}_{1,1} = \mathbf{L}_{2,2} - \mathbf{L}_{1,2}^T \mathbf{L}_{1,1}^{-1} \mathbf{L}_{1,2}$$

- EvalBound** (L^t, t)

- Step 1:** divide N^t nodes in L^t into r and $N^t - r$ nodes.
 - Eigen-decompose $L^t_{1,1}$ to find smallest eigenvalue $\lambda^t_{1,1}$.
 - Perturb L^t by augmented eigenvalue κ^t_{\min}

$$\kappa^t_{\min} = \begin{cases} \lambda^t_1 - \epsilon & \text{if } \lambda^t_1 \leq 0 \\ 0 & \text{o.w.} \end{cases}$$

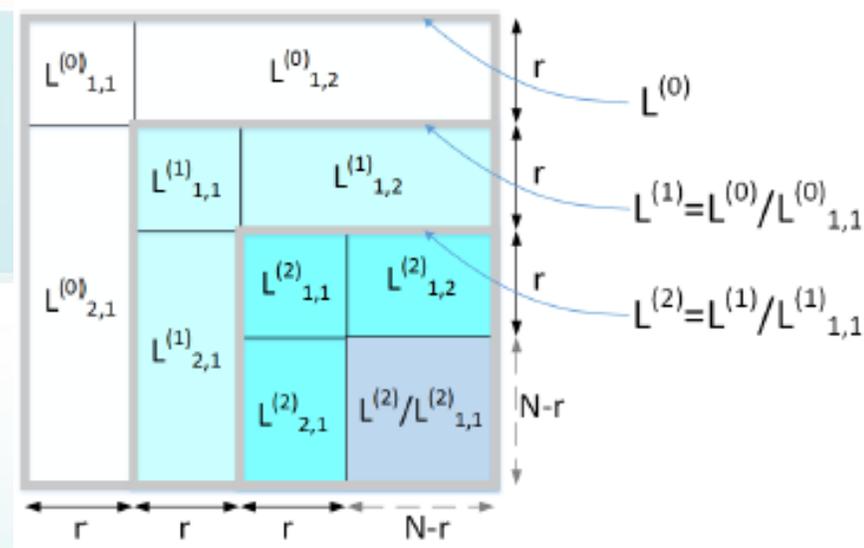
Ensure $L^t_{1,1}$ is PD.



Lower Bound λ_{\min}

- Haysworth Inertia Additivity:

$$\text{In}(\mathbf{L}) = \text{In}(\mathbf{L}_{1,1}) + \text{In}(\mathbf{L}/\mathbf{L}_{1,1})$$



- **Step 2:** ensure SC of $L^t_{1,1}$ is PSD: $\mathcal{L}^t / \mathcal{L}^t_{1,1} = \mathcal{L}^t_{2,2} - (\mathbf{L}^t_{1,2})^T (\mathcal{L}^t_{1,1})^{-1} \mathbf{L}^t_{1,2}$

- if $N^t - r \leq r$,

- eigen-decompose $L^t / L^t_{1,1}$ to find smallest eigenvalue λ^t_2 .

- Compute lower bound: $\lambda^t_{\min} := \kappa^t_{\min} + \min(\lambda^t_2, 0)$

- if $N^t - r > r$,

- Define $\mathbf{L}^{t+1} := \mathcal{L}^t / \mathcal{L}^t_{1,1}$

- Recursively call $\eta^t_{\min} := \text{EvalBound}(\mathbf{L}^{t+1}, t + 1)$

- Return $\lambda^t_{\min} := \kappa^t_{\min} + \eta^t_{\min}$

Complexity $O(N^2 r)$.

IRLS Optimization

- MAP formulation:

$$\min_{\mathbf{x}} \|\mathbf{y} - \mathbf{H}\mathbf{x}\|_0 \gamma + \sigma_0^{-2} \mathbf{x}^T \mathbf{L}_g \mathbf{x}$$

- **Iterative Recursive Least Square** (IRLS) [1]:

- Replace L0-norm with weighted L2-norm, solve iteratively.

$$\min_{\mathbf{x}} (\mathbf{y} - \mathbf{H}\mathbf{x})^T \mathbf{B} (\mathbf{y} - \mathbf{H}\mathbf{x}) \gamma + \sigma_0^{-2} \mathbf{x}^T \mathbf{L}_g \mathbf{x}$$

diagonal matrix w/ weights b 's

$$b_i^{(t+1)} = \frac{1}{(y_i - \mathbf{H}_{i,:}\mathbf{x}^{(t)})^2 + \epsilon}$$

mimics L0-norm

- Sparse linear system of equations:

$$(\gamma \mathbf{H}^T \mathbf{B} \mathbf{H} + \sigma_0^{-2} \mathbf{L}_g) \mathbf{x}^* = \gamma \mathbf{H}^T \mathbf{B}^T \mathbf{y}$$

- Solve via *conjugate gradient* instead of matrix inversion.

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Experimental Setup

- KEEL database [1], face gender dataset [2].
- Features extracted for each sample; ex., local binary pattern (LBP).
- 70% / 30% are training / testing data.
- Graph construction:
 - kNN for positive edges (k=3).
 - Centroid / boundary-based negative edges.
- **Comparison schemes:**
 1. Linear SVM, SVM with RBF kernel
 2. RobustBoost
 3. Graph-Pos, Graph-MinNorm
 4. Graph-Bandlimited, Graph-AdjSmooth, Graph-Wavelet

[1] J. A.-F. et al., “Keel: A software tool to assess evolutionary algorithms to data mining problems,” *Soft Computing*, vol. 13, no.3, February 2009, pp. 307–318.

[2] L. Spacek, “Face recognition data, university of essex, uk,” <http://cswww.essex.ac.uk/mv/allfaces/faces94.html>, Feb. 2007.

Experimental Results

- Comparisons w/ other classifiers:

TABLE I
CLASSIFICATION ERROR RATES IN THE PHONEME DATASET FOR
COMPETING SCHEMES UNDER DIFFERENT TRAINING LABEL ERROR RATES
(THE NUMBERS IN THE PARENTHESES OF THE LAST ROW INDICATE THE
REJECTION RATES)

% label noise	0%	5%	10%	15%	20%
SVM-Linear	21.83%	23.35%	24.55%	25.05%	25.64%
SVM-RBF	16.63%	16.84%	17.48%	17.72%	19.34%
RobustBoost [26]	12.81%	14.91%	17.94%	19.33%	21.50%
Graph-Pos	13.22%	14.91%	16.79%	18.17%	20.70%
Graph-MinNorm	12.90%	14.53%	16.58%	18.45%	20.56%
Graph-Bandlimited [58]	11.70%	14.06%	17.05%	18.70%	21.29%
Graph-AdjSmooth [9]	11.31%	13.69%	16.79%	18.65%	20.67%
Graph-Wavelet [6]	27.25%	28.84%	30.48%	31.95%	33.51%
Proposed-Centroid	10.81%	13.09%	16.18%	17.87%	20.47%
Proposed-Boundary	12.14%	14.44%	17.18%	19.02%	21.51%
Proposed-Hybrid	10.57%	13.00%	15.44%	17.14%	19.15%
Proposed-Rej	9.85% (9.44%)	11.53% (9.69%)	13.97% (9.46%)	14.96% (9.81%)	17.03% (9.80%)

Experimental Results

- Comparisons w/ other classifiers:

TABLE II
CLASSIFICATION ERROR RATES IN THE BANANA DATASET FOR
COMPETING SCHEMES UNDER DIFFERENT TRAINING LABEL ERROR RATES
(THE NUMBERS IN THE PARENTHESES OF THE LAST ROW INDICATE THE
REJECTION RATES)

% label noise	0%	5%	10%	15%	20%
SVM-Linear	54.71%	54.97%	54.70%	53.95%	53.42%
SVM-RBF	12.49%	13.27%	13.72%	16.23%	18.63%
RobustBoost [26]	20.42%	22.73%	24.53%	25.12%	27.52%
Graph-Pos	14.05%	15.89%	18.02%	20.76%	21.93%
Graph-MinNorm	10.23%	12.37%	14.44%	17.41%	18.69%
Graph-Bandlimited [58]	7.53%	11.77%	15.80%	19.14%	21.07%
Graph-AdjSmooth [9]	8.85%	12.08%	15.28%	18.26%	20.67%
Graph-Wavelet [6]	23.18%	24.25%	25.70%	27.15%	30.13%
Proposed-Centroid	5.17%	10.50%	13.79%	16.80%	19.39%
Proposed-Boundary	13.37%	15.68%	18.27%	20.51%	22.72%
Proposed-Hybrid	5.36%	9.43%	12.79%	16.04%	18.43%
Proposed-Rej	3.74%	6.57%	9.26%	12.19%	14.06%
	(9.59%)	(9.89%)	(9.14%)	(9.96%)	(9.95%)

Experimental Results

- Comparisons w/ other classifiers:

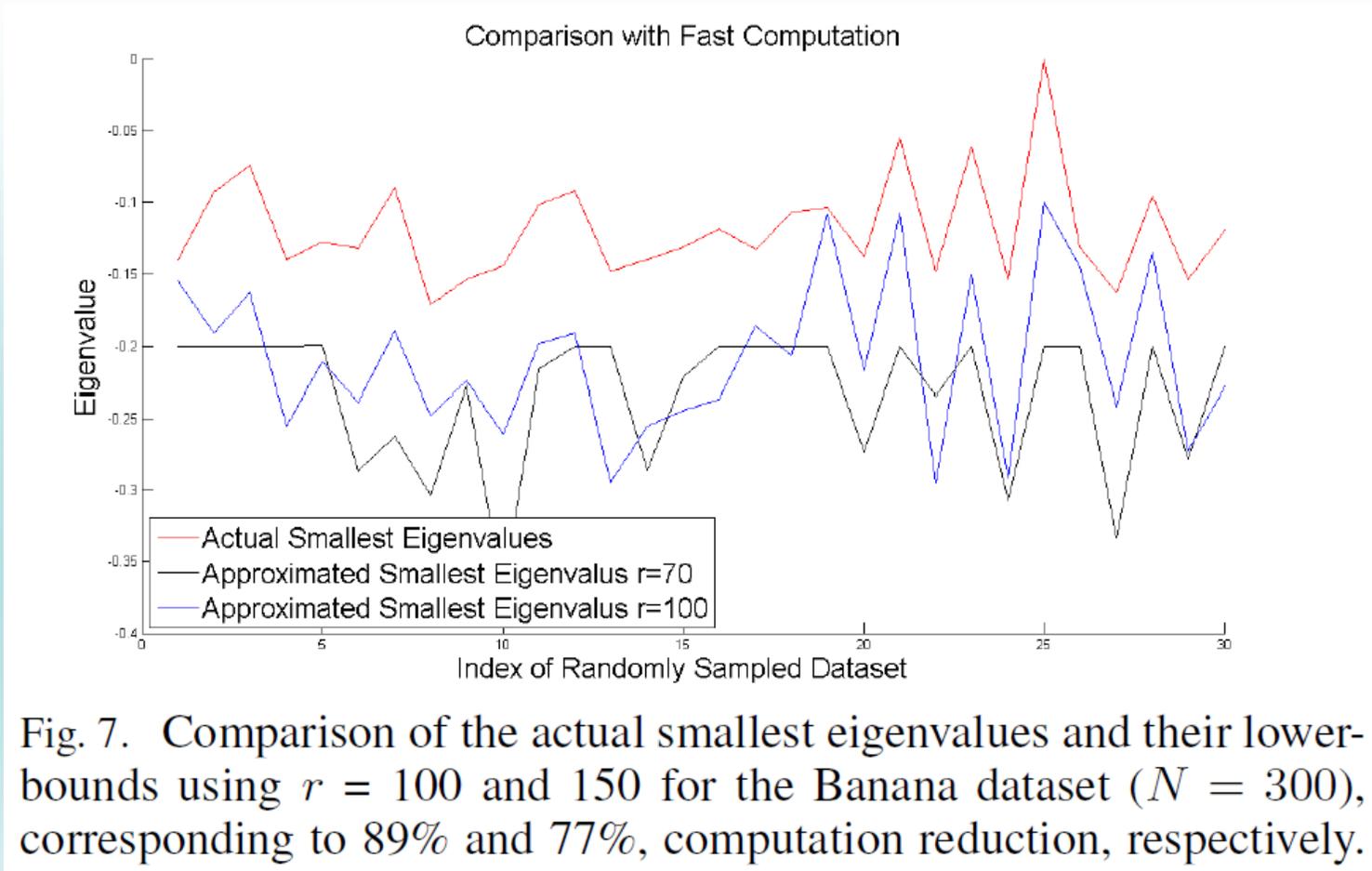
TABLE III

**CLASSIFICATION ERROR RATES IN THE FACE GENDER DATASET FOR
COMPETING SCHEMES UNDER DIFFERENT TRAINING LABEL ERROR RATES
(THE NUMBERS IN THE PARENTHESES OF THE LAST ROW INDICATE THE
REJECTION RATES)**

% label noise	0%	5%	10%	15%	20%
SVM-Linear	17.65%	18.22%	18.77%	19.59%	21.6%
SVM-RBF	12.14%	12.16%	12.83%	16.30%	24.01%
RobustBoost [26]	9.15%	11.09%	14.36%	17.36%	20.68%
Graph-Pos	13.15%	13.62%	14.38%	15.39%	16.54%
Graph-MinNorm	7.15%	8.26%	9.48%	10.37%	12.01%
Graph-Bandlimited [58]	5.78%	11.83%	15.30%	19.74%	23.44%
Graph-AdjSmooth [9]	1.25%	5.01%	7.94%	11.45%	15.39%
Graph-Wavelet [6]	20.02%	19.95%	20.12%	20.7%	21.43%
Proposed-Centroid	1.44%	2.96%	4.46%	5.88%	8.07%
Proposed-Boundary	10.81%	12.09%	13.17%	14.33%	15.96%
Proposed-Hybrid	1.71%	3.02%	4.22%	5.75%	7.71%
Proposed-Rej	0.36% (9.70%)	0.68% (9.29%)	1.08% (9.85%)	2.39% (9.08%)	4.18% (9.05%)

Experimental Results

- λ_{\min} versus computed lower bound:



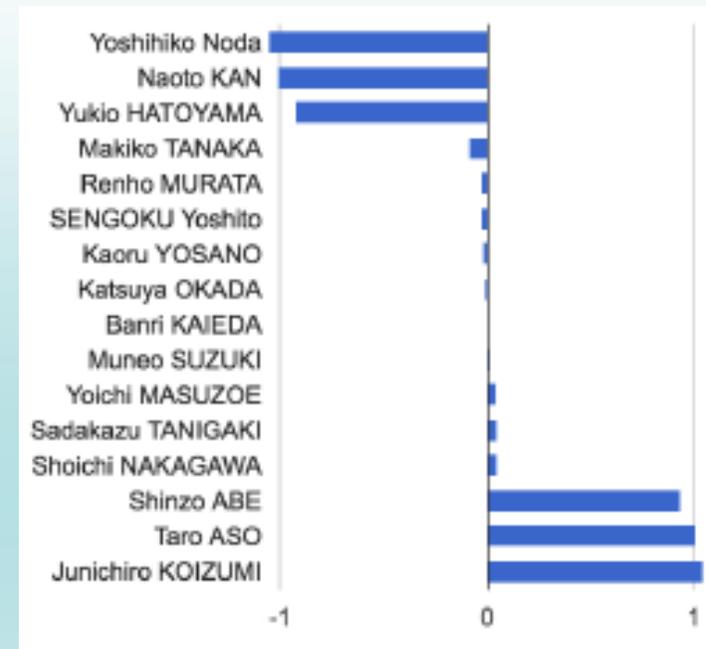
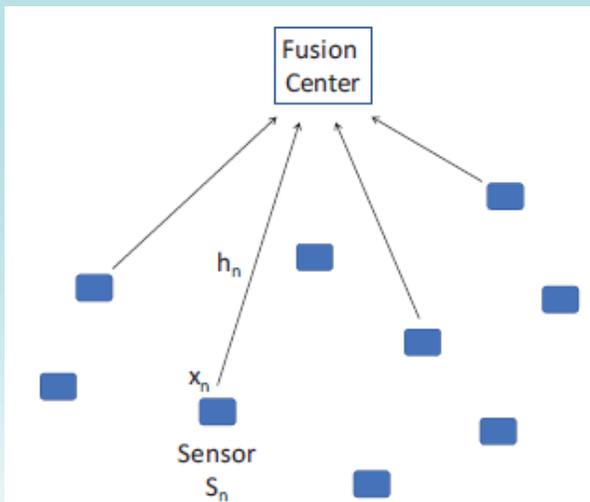
Conclusion

- Graph Signal Processing (GSP)
 - Tools to process signals that live on graphs.
- Graph-based binary classifier
 - Similarity graph with +/- edges, given features.
 - Perturbed graph Laplacian that is PSD.
 - Fast computation of min eigenvalue lower bound.
 - Fast MAP solver via IRLS, conjugate gradient.

Other GSP Works

- Coding of LF, spectral image [1], 3D point cloud w/ GFT.
- Coding of graph data w/ graph wavelets.
- Political leaning estimation [2].
- Wireless signal / power estimation [3].

[1] J. Zeng, G. Cheung, Y.-H. Chao, I. Blanes, J. Serra-Sagrsta, A. Ortega, "**Hyperspectral Image Coding using Graph Wavelets**," accepted to *IEEE International Conference on Image Processing*, Beijing, China, September, 2017.



[2] B. Renoust et al., "**Estimation of Political Leanings via Graph-Signal Restoration**," submitted to *IEEE International Conference on Acoustics, Speech and Signal Processing*, New Orleans, USA, March, 2017

[3] M. Kaneko, G. Cheung, W.-t. Su, C.-W. Lin, "**Graph-based Joint Signal / Power Restoration for Energy Harvesting Wireless Sensor Networks**," submitted to *IEEE Globecom*, Singapore, December, 2017.

Q&A

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