

Graph Signal Processing

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Network as graph G(V, E): encode pairwise relationships

- Desiderata: Process, analyze and learn from network data [Kolaczyk'09]
 ⇒ Use G to study graph signals, data associated with nodes in V
- Ex: Opinion profile, buffer congestion levels, neural activity, epidemic



Graph signal processing: Motivation and fundamentals

Learning graphs from observations of smooth signals

Case study: Discriminative graph learning for emotion recognition

Graph signal processing (GSP)



Graph G with adjacency matrix A
 ⇒ A_{ij} = proximity between i and j
 Signal x ∈ ℝ^{N_v} on top of the graph
 ⇒ x_i = signal value at node i



- ▶ Graph Signal Processing \rightarrow Exploit structure encoded in **A** to process **x**
- Q: Graph signals common and interesting as networks are?
- Q: Why do we expect the graph structure to be useful in processing x?

A. Ortega et al, "Graph signal processing: Overview, challenges, and applications," *Proc. IEEE*, 2018



- Bureau of Economic Analysis of the U.S. Department of Commerce
 - $A_{ij} =$ Output of sector *i* that becomes input to sector *j* (62 sectors)



- Oil extraction (OG), Petroleum and coal products (PC), Construction (CO)
- Administrative services (AS), Professional services (MP)
- Credit intermediation (FR), Securities (SC), Real state (RA), Insurance (IC)
- Only interactions stronger than a threshold are shown



Bureau of Economic Analysis of the U.S. Department of Commerce
 A_{ij} = Output of sector *i* that becomes input to sector *j* (62 sectors)



- A few sectors have widespread strong influence (services, finance, energy)
- Some sectors have strong indirect influences (oil)
- The heavy last row is final consumption
- This is an interesting network \Rightarrow Signals on this graph are as well



Signal x = output per sector = disaggregated GDP

 \Rightarrow Network structure used to, e.g., reduce GDP estimation noise



Signal is as interesting as the network itself. Arguably more

- Same is true for brain connectivity and fMRI brain signals, ...
- Gene regulatory networks and gene expression levels, ...
- Online social networks and information cascades, ...

Signal and Information Processing is about exploiting signal structure

- ► Discrete time described by cyclic graph ⇒ Time *n* follows time *n* − 1
 - \Rightarrow Signal value x_n similar to x_{n-1}
- Formalized with the notion of frequency



► Fourier transform ⇒ Projection on eigenvector space of cycle







► Random signal with mean E [x] = 0 and covariance C_x = E [xx^H] ⇒ Eigenvector decomposition C_x = VAV^H

Covariance matrix A = C_x is a graph
 ⇒ Not a very good graph, but still

Precision matrix C_x⁻¹ a common graph too
 ⇒ Conditional dependencies of Gaussian x



► Covariance matrix structure \Rightarrow Principal components (PCA) $\Rightarrow \tilde{\mathbf{x}} = \mathbf{V}^H \mathbf{x}$

- ▶ PCA transform ⇒ Projection on eigenvector space of (inverse) covariance
- Q: Can we extend these principles to general graphs and signals?



- ► Adjacency **A**, Laplacian **L**, or, generically graph shift $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$ $\Rightarrow S_{ij} = 0$ for $i \neq j$ and $(i, j) \notin E$ (captures local structure in *G*)
- ► The Graph Fourier Transform (GFT) of x is defined as

$$ilde{\mathsf{x}} = \mathsf{V}^{-1}\mathsf{x}$$

▶ While the inverse GFT (iGFT) of x̃ is defined as

$\mathbf{x} = \mathbf{V} \tilde{\mathbf{x}}$

 \Rightarrow Eigenvectors $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_{N_v}]$ are the frequency basis (atoms)

Additional structure

 \Rightarrow If **S** is normal, then $\mathbf{V}^{-1} = \mathbf{V}^H$ and $\tilde{x}_k = \mathbf{v}_k^H \mathbf{x} = \langle \mathbf{v}_k, \mathbf{x} \rangle$

 \Rightarrow Parseval holds, $\|\mathbf{x}\|^2 = \|\mathbf{\tilde{x}}\|^2$

► GFT ⇒ Projection on eigenvector space of graph shift operator S

Frequency modes of the Laplacian



► Total variation of signal x with respect to L

$$\mathsf{TV}(\mathbf{x}) = \mathbf{x}^{\top} \mathsf{L} \mathbf{x} = \sum_{i,j=1,j>i}^{N_v} A_{ij} (x_i - x_j)^2$$

⇒ Smoothness measure on the graph G (Dirichlet energy)
For Laplacian eigenvectors V = [v₁,..., v_{N_v}] ⇒ TV(v_k) = λ_k ⇒ Can view 0 = λ₁ < ··· ≤ λ_{N_v} as frequencies
Ex: gene network, N_v=10, k=1, k=2, k=9



- ▶ Particularized to cyclic graphs \Rightarrow GFT \equiv Fourier transform
- Also for covariance graphs \Rightarrow GFT \equiv PCA transform
- ▶ But really, this is an empirical question. GFT of disaggregated GDP



► Spectral domain representation characterized by a few coefficients ⇒ Notion of bandlimitedness: $\mathbf{x} = \sum_{k=1}^{K} \tilde{x}_k \mathbf{v}_k$ ⇒ Sampling, compression, filtering, pattern recognition



GFT of brain signals during a visual-motor learning task [Huang et al'16]
 Decomposed into low, medium and high frequency components



Brain: Complex system where regularity coexists with disorder [Sporns'11]
 ⇒ Signal energy mostly in the low and high frequencies
 ⇒ In brain regions akin to the visual and sensorimotor cortices



- Learning graphs from nodal observations
- Key in neuroscience
 - \Rightarrow Functional network from fMRI signals



- ▶ Most GSP works: how known graph **S** affects signals and filters
- ▶ Here, reverse path: how to use GSP to infer the graph topology?
 - Graphical models [Egilmez et al'16], [Rabbat'17], [Kumar et al'19], ...
 - Smooth signals [Dong et al'15], [Kalofolias'16], [Sardellitti et al'17], ...
 - ▶ Graph filtering models [Shafipour et al'17], [Thanou et al'17], ...
 - Stationary signals [Pasdeloup et al'15], [Segarra et al'16], ...
 - Directed graphs [Mei-Moura'15], [Shen et al'16], ...







In Deduction Medices data analysis and preserving tails typically invol-large uris of simultaneil data, where the structure carries cell

100000 (Marcala)

Topology Identification and Learning Over Graphs: Accounting for Nonlinearities and Dynamics

This article focuses on the problem of learning graphs from data, in particular, to capture the nonlinear and dynamic dependencies.

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Recent tutorials on learning graphs from data (with a GSP flavor) IEEE Signal Processing Magazine and Proceedings of the IEEE



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Problem formulation

Rationale

- Seek graphs on which data admit certain regularities
 - Nearest-neighbor prediction (a.k.a. graph smoothing)
 - Semi-supervised learning
 - Efficient information-processing transforms
- Many real-world graph signals are smooth
 - Graphs based on similarities among vertex attributes
 - Network formation driven by homophily, proximity in latent space

Problem statement

Given observations $\mathcal{X} := {\mathbf{x}_p}_{p=1}^P$, identify a graph G such that signals in \mathcal{X} are smooth on G.

Criterion: Dirichlet energy on the graph G with Laplacian L

$$\mathsf{TV}(\mathsf{x}) = \mathsf{x}^{\top}\mathsf{L}\mathsf{x}$$





Baker's yeast data, formally known as *Saccharomyces cerevisiae*

▶ Graph: 134 vertices (proteins) and 241 edges (protein interactions)



Signal: functional annotation intracellular signaling cascade (ICSC)

- Signal transduction, how cells react to the environment
- ▶ $x_i = 1$ if protein *i* annotated ICSC (yellow), $x_i = 0$ otherwise (blue)

Example: Predicting law practice



Working relationships among lawyers [Lazega'01]

Graph: 36 partners, edges indicate partners worked together



Signal: various node-level attributes $\mathbf{x} = \{x_i\}_{i \in V}$ including

 \Rightarrow Type of practice, i.e., litigation (red) and corporate (cyan)

Suspect lawyers collaborate more with peers in same legal practice

 \Rightarrow Knowledge of collaboration useful in predicting type of practice



Consider an unknown graph G with Laplacian L = VΛV[⊤] ⇒ Adopt GFT basis V as signal representation matrix

► Factor analysis model for the observed graph signal

 $\mathbf{x} = \mathbf{V} \boldsymbol{\chi} + \boldsymbol{\epsilon}$

 \Rightarrow Latent variables $\chi \sim \mathcal{N}(\mathbf{0}, \mathbf{\Lambda}^{\dagger}) \ (\approx$ GFT coefficients)

 \Rightarrow Isotropic error term $\boldsymbol{\epsilon} \sim \mathcal{N}(\mathbf{0}, \sigma^2 \mathbf{I})$

- Smoothness: prior encourages low-pass bandlimited x
 - \Rightarrow Small eigenvalues of L (low freq.) \rightarrow High-power factor loadings

X. Dong et al, "Learning Laplacian matrix in smooth graph signal representations," *IEEE Trans. Signal Process.*, 2016



 \blacktriangleright Maximum a posteriori (MAP) estimator of the latent variables χ

$$\hat{\boldsymbol{\chi}}_{\mathsf{MAP}} = \arg\min_{\boldsymbol{\chi}} \left\{ \| \mathbf{x} - \mathbf{V} \boldsymbol{\chi} \|^2 + \alpha \boldsymbol{\chi}^\top \mathbf{\Lambda} \boldsymbol{\chi} \right\}$$

 \Rightarrow Parameterized by the unknown ${\bm V}$ and ${\bm \Lambda}$

• Define predictor $\mathbf{y} := \mathbf{V} \boldsymbol{\chi}$, regularizer expressible as

$$\boldsymbol{\chi}^{\top} \boldsymbol{\Lambda} \boldsymbol{\chi} = \boldsymbol{\mathsf{y}}^{\top} \boldsymbol{\mathsf{V}} \boldsymbol{\Lambda} \boldsymbol{\mathsf{V}}^{\top} \boldsymbol{\mathsf{y}} = \boldsymbol{\mathsf{y}}^{\top} \boldsymbol{\mathsf{L}} \boldsymbol{\mathsf{y}} = \mathsf{T} \mathsf{V}(\boldsymbol{\mathsf{y}})$$

 \Rightarrow Laplacian-based TV denoiser of **x**, smoothness prior on **y**

 \Rightarrow Kernel-ridge regression with unknown **K** := **L**[†] (graph filter)

Idea: jointly search for **L** and denoised representation $\mathbf{y} = \mathbf{V} \boldsymbol{\chi}$

$$\min_{\mathbf{L},\mathbf{y}} \left\{ \|\mathbf{x} - \mathbf{y}\|^2 + \alpha \mathbf{y}^\top \mathbf{L} \mathbf{y} \right\}$$



▶ Given signals
$$\mathcal{X} := \{\mathbf{x}_{\rho}\}_{\rho=1}^{P}$$
 in $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_P] \in \mathbb{R}^{N_v \times P}$, solve

$$\min_{\mathbf{L},\mathbf{Y}} \left\{ \|\mathbf{X} - \mathbf{Y}\|_{F}^{2} + \alpha \operatorname{trace}\left(\mathbf{Y}^{\top}\mathbf{L}\mathbf{Y}\right) + \frac{\beta}{2}\|\mathbf{L}\|_{F}^{2} \right\}$$

s. to
$$\operatorname{trace}(\mathbf{L}) = N_{v}, \ \mathbf{L}\mathbf{1} = \mathbf{0}, \ L_{ij} = L_{ji} \leq 0, \ i \neq j$$

 $\Rightarrow \mbox{Objective function: Fidelity} + \mbox{smoothness} + \mbox{edge sparsity} \\ \Rightarrow \mbox{Not jointly convex in } L \mbox{ and } Y, \mbox{ but bi-convex} \\$

• Algorithmic approach: alternating minimization (AM), $O(N_v^3)$ cost (S1) Fixed Y: solve for L via interior-point method, ADMM (more soon) (S2) Fixed L: low-pass, graph filter-based smoother of the signals in X $Y = (I + \alpha L)^{-1} X$



• Generate multiple signals on a synthetic Erdős-Rényi graph \Rightarrow Recover the graph for different values of α and β



- More edges promoted by increasing β and decreasing α
- ▶ In the low noise regime, the ratio β/α determines behavior



- ▶ $N_v = 89$ stations measuring monthly temperature averages (1981-2010)
 - \Rightarrow Learn a graph G on which the temperatures vary smoothly
- ► Geographical distance not a good idea ⇒ different altitudes



▶ Recover altitude partition from spectral clustering on G
 ⇒ Red (high stations) and blue (low stations) clusters
 ▶ K-means applied directly to the temperatures (right) fails

Signal smoothness meets edge sparsity



▶ Recall $\mathbf{X} = [\mathbf{x}_1, \dots, \mathbf{x}_P] \in \mathbb{R}^{N_v \times P}$, let $\bar{\mathbf{x}}_i^\top \in \mathbb{R}^{1 \times P}$ denote its *i*-th row ⇒ Euclidean distance matrix $\mathbf{Z} \in \mathbb{R}_+^{N_v \times N_v}$, where $Z_{ij} := \|\bar{\mathbf{x}}_i - \bar{\mathbf{x}}_j\|^2$

Neat trick: link between smoothness and sparsity

$$\sum_{\rho=1}^{P} \mathsf{TV}(\mathbf{x}_{\rho}) = \mathsf{trace}(\mathbf{X}^{\top} \mathbf{L} \mathbf{X}) = \frac{1}{2} \| \mathbf{A} \circ \mathbf{Z} \|_{1}$$

 \Rightarrow Sparse *E* when data come from a smooth manifold

 \Rightarrow Favor candidate edges (i, j) associated with small Z_{ij}

Shows that edge sparsity on top of smoothness is redundant

Parameterize graph learning problems in terms of A (instead of L)
 Advantageous since constraints on A are decoupled

V. Kalofolias, "How to learn a graph from smooth signals," *AISTATS*, 2016



General purpose model for learning graphs [Kalofolias'16]

$$\begin{split} \min_{\mathbf{A}} & \left\{ \|\mathbf{A} \circ \mathbf{Z}\|_1 - \alpha \mathbf{1}^\top \log(\mathbf{A}\mathbf{1}) + \frac{\beta}{2} \|\mathbf{A}\|_F^2 \right\} \\ \text{s. to} & \text{diag}(\mathbf{A}) = \mathbf{0}, \ A_{ij} = A_{ji} \geq 0, \ i \neq j \end{split}$$

 \Rightarrow Logarithmic barrier forces positive degrees

\Rightarrow Penalize large edge-weights to control sparsity

- Primal-dual solver amenable to parallelization, $O(N_v^2)$ cost
- Laplacian-based factor analysis encore. Tackle (S1) as

$$\begin{split} \min_{\mathbf{A}} & \left\{ \|\mathbf{A} \circ \mathbf{Z}\|_1 - \log(\mathbb{I}\left\{\|\mathbf{A}\|_1 = N_v\right\}) + \frac{\beta}{2} \left(\|\mathbf{A}\mathbf{1}\|^2 + \|\mathbf{A}\|_F^2\right) \right\}\\ \text{s. to} \quad \text{diag}(\mathbf{A}) = \mathbf{0}, \ A_{ij} = A_{ji} \geq 0, \ i \neq j \end{split}$$

Example: Learning the graph of USPS digits



- ▶ 1001 images of the 10 digits, but highly imbalanced (2.6*i*²)
 ⇒ 10 classes via graph recovery plus spectral clustering
- Compare two methods based on smoothness and k-NN graph



Performance more robust to graph density

 \Rightarrow Likely attributable to non-singleton nodes



- Idea: parameterize the unknown topology via an edge indicator vector
- ► Complete graph on N_V nodes, having $M := \binom{N_v}{2}$ edges ⇒ Incidence matrix $\mathbf{B} := [\mathbf{b}_1, \dots, \mathbf{b}_M] \in \mathbb{R}^{N_v \times M}$

• Laplacian of a candidate graph G(V, E)

$$\mathbf{L}(\boldsymbol{\omega}) = \sum_{m=1}^{M} \omega_m \mathbf{b}_m \mathbf{b}_m^{\top}$$

⇒ Binary edge indicator vector $\boldsymbol{\omega} := [\omega_1, \dots, \omega_M]^\top \in \{0, 1\}^M$ ⇒ Offers an explicit handle on the number of edges $\|\boldsymbol{\omega}\|_0 = |E|$

Problem: Given observations $\mathcal{X} := {\mathbf{x}_p}_{p=1}^{P}$, learn an unweighted graph G(V, E) such that signals in \mathcal{X} are smooth on G and |E| = K.

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Natural formulation is to solve the non-convex problem

$$\min_{oldsymbol{\omega}\in\{0,1\}^M} ext{trace}(oldsymbol{X}^{ op}oldsymbol{\mathsf{L}}(oldsymbol{\omega})oldsymbol{\mathsf{X}}), ext{ s. to } \|oldsymbol{\omega}\|_0=K$$

Solution obtained through a simple rank-ordering procedure

- Compute edge scores $c_m := \text{trace}(\mathbf{X}^{\top}(\mathbf{b}_m \mathbf{b}_m^{\top})\mathbf{X})$
- Set $\omega_m = 1$ for those K edges having the smallest scores

▶ More pragmatic AWGN setting where $\mathbf{x}_p = \mathbf{y}_p + \boldsymbol{\epsilon}_p$, $p = 1, \dots, P$

$$\min_{\mathbf{Y},\boldsymbol{\omega}\in\{0,1\}^M}\left\{\|\mathbf{X}-\mathbf{Y}\|_F^2 + \alpha \mathsf{trace}(\mathbf{Y}^{\top}\mathbf{L}(\boldsymbol{\omega})\mathbf{Y})\right\}, \quad \mathsf{s. to} \ \|\boldsymbol{\omega}\|_0 = K$$

\Rightarrow Tackle via AM or semidefinite relaxation (SDR)

S. Chepuri et al, "Learning sparse graphs under smoothness prior," *ICASSP*, 2017

Comparative summary



Noteworthy features of the edge subset selection approach

- $\checkmark\,$ Direct control on edge sparsity
- $\checkmark\,$ Simple algorithm in the noise-free case
- ✓ Devoid of Laplacian feasibility constraints
- \checkmark Does not guarantee connectivity of G
- X No room for optimizing edge weights

Scalable framework in [Kalofolias'16] also quite flexible

$$\begin{split} \min_{\mathbf{A}} \left\{ \|\mathbf{A} \circ \mathbf{Z}\|_1 + g(\mathbf{A}) \right\} \\ \text{s. to} \quad \text{diag}(\mathbf{A}) = \mathbf{0}, \ A_{ij} = A_{ji} \geq 0, \ i \neq j \end{split}$$

 \Rightarrow Subsumes the factor-analysis model [Dong et al'16]

 \Rightarrow Recovers Gaussian kernel weights $A_{ij} := \exp\left(-\frac{\|ar{\mathbf{x}}_i - ar{\mathbf{x}}_j\|^2}{\sigma^2}
ight)$ for

$$g(\mathbf{A}) = \sigma^2 \sum_{i,j} A_{ij} (\log(A_{ij}) - 1)$$



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► Labeled graph signals $\mathcal{X}_c := \{\mathbf{x}_p^{(c)}\}_{p=1}^{P_c}$ from *C* different classes ⇒ Signals in each class possess a very distinctive structure

▶ As.: Class c signals are smooth w.r.t. unknown $G_c(V, E_c)$

Multiple linear subspace model

 \Rightarrow Signals spanned by few Laplacian modes (GFT components)

 \Rightarrow Like susbpace clustering [Vidal'11], but with supervision

Problem statement

Given training signals $\mathcal{X} = \bigcup_{c=1}^{C} \mathcal{X}_c$, learn discriminative graphs \mathbf{A}_c under smoothness priors to classify test signals via GFT projections.



 \blacktriangleright Discriminative graph learning per class c

$$\min_{\mathbf{A}_{c}} \left\{ \|\mathbf{A}_{c} \circ \mathbf{Z}_{c}\|_{1} - \alpha \mathbf{1}^{\top} \log(\mathbf{A}_{c}\mathbf{1}) + \frac{\beta}{2} \|\mathbf{A}_{c}\|_{F}^{2} - \gamma \sum_{k \neq c}^{C} \|\mathbf{A}_{c} \circ \mathbf{Z}_{k}\|_{1} \right\}$$

s. to $\operatorname{diag}(\mathbf{A}_c) = \mathbf{0}, \ [\mathbf{A}_c]_{ij} = [\mathbf{A}_c]_{ji} \ge 0, \ i \neq j$

 $\Rightarrow Capture the underlying graph topology (class c structure)$ $\Rightarrow Discriminability to boost classification performance$

- Q: Given graphs $\{\hat{\mathbf{A}}_c\}_{c=1}^C$, how do we classify a test signal x?
- Pass x through a filter-bank with C low-pass filters (LPFs)

$$\mathbf{\tilde{x}}_{F,c} = \operatorname{diag}(\mathbf{\tilde{h}})\mathbf{\hat{V}}_{c}^{\top}\mathbf{x} \quad \Rightarrow \quad \hat{c} = \operatorname{argmax}_{c}\left\{\|\mathbf{\tilde{x}}_{F,c}\|^{2}\right\}$$

 \Rightarrow LPF frequency response $\tilde{\mathbf{h}}_{\text{r}}$ learned class-c GFT basis $\hat{\mathbf{V}}_{c}$



- Discriminative graph learning for emotion recognition from EEG signals
- ▶ DEAP dataset \Rightarrow 32 subjects watch music videos (40 trials each)
 - Asked to rate videos: valence, arousal, like/dislike, dominance
 - Focus on valence labels: low (1-5 rating) and high (6-10 rating)
 - Signals acquired from $N_v = 32$ EEG channels
- ► We perform a subject-specific valence classification task
 - \Rightarrow Learn C = 2 graphs and project onto the 8 smoothest modes
 - \Rightarrow Report leave-one (trial)-out classification accuracy
- Mean classification accuracy over subjects is 92.73%

S. S. Saboksayr et al, "Online discriminative graph learning from multi-class smooth signals," *Signal Processing*, 2022

Valence classification





Q: What information do we glean from the class-conditional graphs?



Asymmetric frontal activity apparent from the 8 smoothest modes





- Graph signal
- Graph signal processing
- Fourier transform
- Covariance matrix
- Principal component analysis
- Graph shift operator
- Graph Fourier transform
- Topology identification
- Smooth signal
- Dirichlet energy
- Factor analysis model

- Alternating minimization
- Euclidean distance matrix
- Edge subset selection
- Gaussian kernel graph
- Multiple subspace model
- Subspace clustering
- Discriminative graphs
- Low-pass graph filter
- Emotion recognition
- EEG signals
- Valence classification