

Graph Signal Processing: Foundational Advances For Learning From Network Data

Gonzalo Mateos

Dept. of ECE and Goergen Institute for Data Science

University of Rochester

gmateosb@ece.rochester.edu

<http://www.ece.rochester.edu/~gmateosb/>

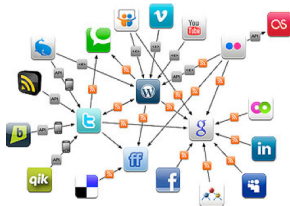
Collaborators: R. Shafipour, S. Segarra, A. G. Marques, and A. Ribeiro

Acknowledgment: NSF Awards CCF-1750428 and ECCS-1809356

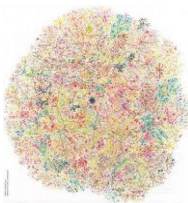
Rochester, NY, October 4, 2019

Network Science analytics

Online social media



Internet



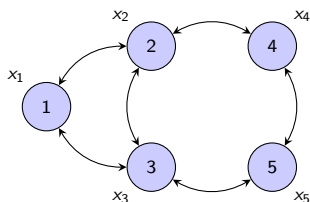
Clean energy and grid analytics



- ▶ **Network as graph** $G = (\mathcal{V}, \mathcal{E})$: encode pairwise relationships
- ▶ **Desiderata**: Process, analyze and learn from **network data** [Kolaczyk'09]
⇒ Use G to study **graph signals**, **data** associated with **nodes** in \mathcal{V}
- ▶ **Ex**: Opinion profile, buffer congestion levels, neural activity, epidemic

Graph signal processing (GSP)

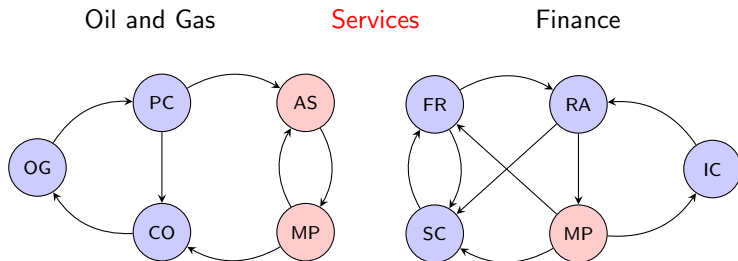
- ▶ Graph G with adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$
 $\Rightarrow A_{ij} = \text{proximity between } i \text{ and } j$
- ▶ Define a signal $\mathbf{x} \in \mathbb{R}^N$ on top of the graph
 $\Rightarrow x_i = \text{signal value at node } i$



- ▶ Graph Signal Processing \rightarrow Exploit structure encoded in \mathbf{A} to process \mathbf{x}
 \Rightarrow Our view: GSP well suited to study (network) diffusion processes
- ▶ Q: Graph signals common and interesting as networks are?
- ▶ Q: Why do we expect the graph structure to be useful in processing \mathbf{x} ?

Network of economic sectors of the United States

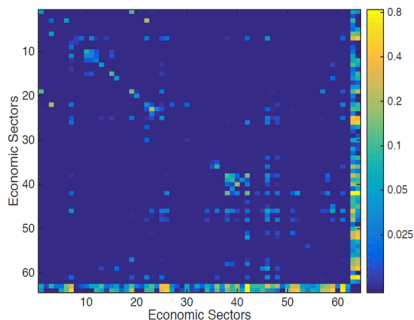
- ▶ Bureau of Economic Analysis of the U.S. Department of Commerce
 - ▶ A_{ij} = Output of sector i that becomes input to sector j (62 sectors)



- ▶ 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

Network of economic sectors of the United States

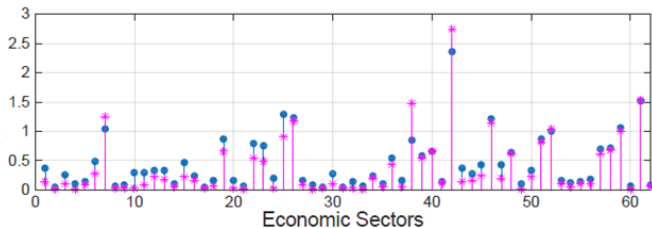
- ▶ Bureau of Economic Analysis of the U.S. Department of Commerce
 - ▶ A_{ij} = Output of sector i that becomes input to sector j (62 sectors)



- ▶ 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

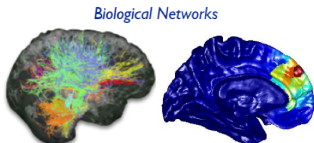
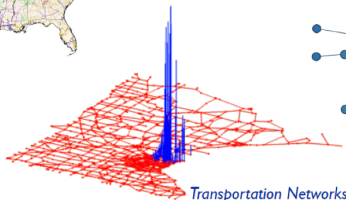
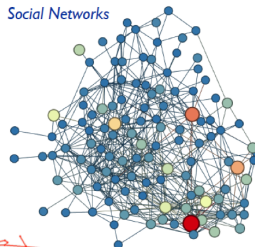
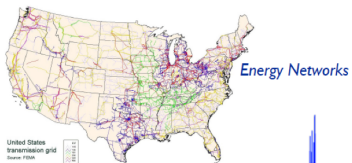
Disaggregated GDP of the United States

- ▶ Signal \mathbf{x} = output per sector = disaggregated GDP
 - ⇒ 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, ...

Graph signals are ubiquitous



© D. Shuman

Importance of signal structure in time

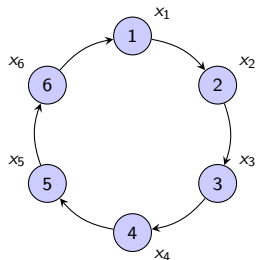
- ▶ Signal and Information Processing **is about exploiting signal structure**

- ▶ Discrete time described by cyclic graph

⇒ Time n follows time $n - 1$

⇒ Signal value x_n similar to x_{n-1}

- ▶ Formalized with the notion of frequency



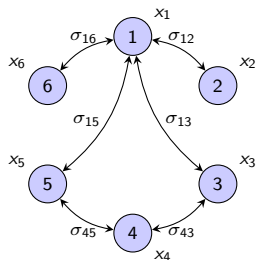
- ▶ Cyclic structure ⇒ Fourier transform ⇒ $\tilde{\mathbf{x}} = \mathbf{F}^H \mathbf{x}$ $\left(F_{kn} = \frac{e^{j2\pi kn/N}}{\sqrt{N}} \right)$

- ▶ **Fourier transform** ⇒ **Projection on eigenvector space of cycle**

Covariances and principal components

- ▶ Random signal with mean $\mathbb{E}[\mathbf{x}] = 0$ and covariance $\mathbf{C}_x = \mathbb{E}[\mathbf{x}\mathbf{x}^H]$
 - ⇒ Eigenvector decomposition $\mathbf{C}_x = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$

- ▶ Covariance matrix $\mathbf{A} = \mathbf{C}_x$ is a graph
 - ⇒ Not a very good graph, but still
- ▶ Precision matrix \mathbf{C}_x^{-1} a common graph too
 - ⇒ Conditional dependencies of Gaussian \mathbf{x}



- ▶ Covariance matrix structure ⇒ Principal components (PCA) ⇒ $\tilde{\mathbf{x}} = \mathbf{V}^H \mathbf{x}$
- ▶ **PCA transform** ⇒ Projection on eigenvector space of (inverse) covariance
- ▶ **Q:** Can we extend these principles to general graphs and signals?

Graph Fourier Transform

- ▶ Adjacency \mathbf{A} , Laplacian \mathbf{L} , or, generically **graph shift** $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$
 $\Rightarrow S_{ij} = 0$ for $i \neq j$ and $(i, j) \notin \mathcal{E}$ (captures local structure in G)

- ▶ The **Graph Fourier Transform (GFT)** of \mathbf{x} is defined as

$$\tilde{\mathbf{x}} = \mathbf{V}^{-1}\mathbf{x}$$

- ▶ While the **inverse GFT (iGFT)** of $\tilde{\mathbf{x}}$ is defined as

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

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

- ▶ Additional structure

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

- ▶ **GFT** \Rightarrow **Projection on eigenvector space of graph shift operator \mathbf{S}**

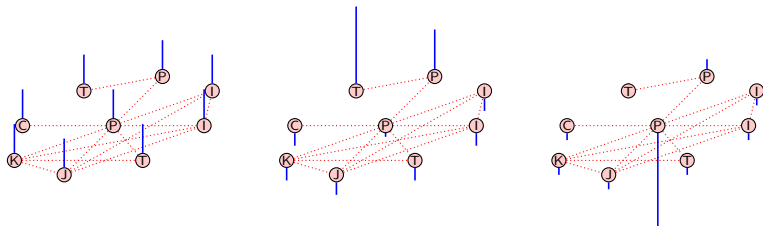
Frequency modes of the Laplacian

- ▶ **Total variation** of signal \mathbf{x} with respect to \mathbf{L}

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

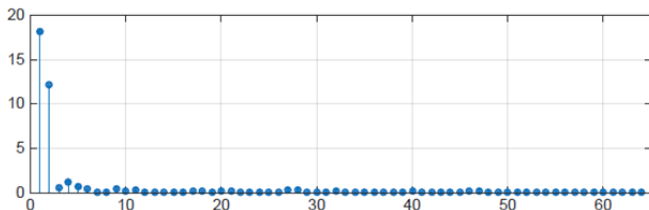
⇒ Smoothness measure on the graph G (Dirichlet energy)

- ▶ For Laplacian eigenvectors $\mathbf{V} = [\mathbf{v}_1, \dots, \mathbf{v}_N]$ ⇒ $\text{TV}(\mathbf{v}_k) = \lambda_k$
⇒ Can view $0 = \lambda_1 < \dots \leq \lambda_N$ as frequencies
- ▶ **Ex:** gene network, $N=10$, $k=1$, $k=2$, $k=9$



Is this a reasonable transform?

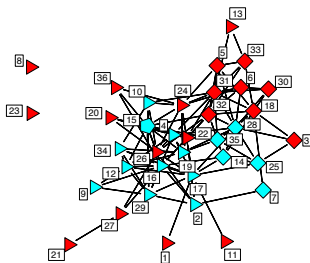
- ▶ Particularized to cyclic graphs \Rightarrow GFT \equiv Fourier transform
- ▶ Also for covariance graphs \Rightarrow GFT \equiv PCA transform
- ▶ But really, this is an **empirical question**. GFT of disaggregated GDP



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

Predicting law practice

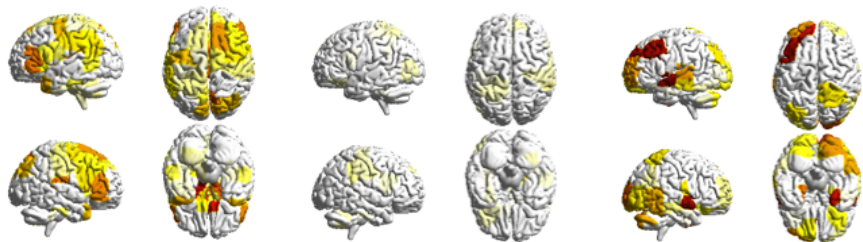
- ▶ Working relationships among lawyers [Lazega'01]
 - ▶ **Graph:** 36 partners, edges indicate partners worked together



- ▶ **Signal:** various node-level attributes $\mathbf{x} = \{x_i\}_{i \in \mathcal{V}}$ including
 - ⇒ Type of practice, i.e., litigation (red) and corporate (cyan)
- ▶ Suspect lawyers collaborate more with peers in same legal practice
 - ⇒ Knowledge of collaboration useful in predicting type of practice

Graph frequency analysis of brain signals

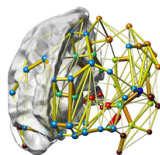
- ▶ GFT of brain signals during a **visual-motor learning task** [Huang et al'16]
 - ⇒ Decomposed into low, medium and high frequency components



- ▶ 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

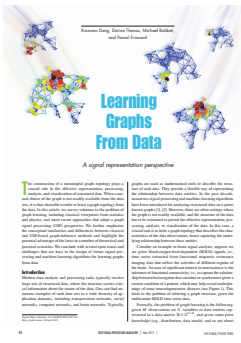
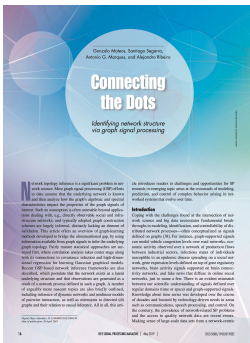
Learning graphs from data

- ▶ **Learning graphs** from nodal observations
- ▶ Key in neuroscience
 - ⇒ Functional network from fMRI signals
- ▶ Most GSP works: how known graph \mathbf{S} affects signals and filters
- ▶ Here, reverse path: how to use **GSP to infer the graph topology**?
 - ▶ Gaussian graphical models [Egilmez et al'16], [Rabbat'17], ...
 - ▶ 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 [Paseloup et al'15], [Segarra et al'16], ...
 - ▶ Directed graphs [Mei-Moura'15], [Shen et al'16], ...



Connecting the dots

- ▶ Recent **tutorials** on learning graphs from data
- ▶ IEEE Signal Processing Magazine and Proceedings of the IEEE



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 dependence.

By GIORGIO B. GIANNAKI¹, FALHA ISLAM², YANFANG BAO³, Student Member IEEE, AND GIORGINO VULIARI KARAKULAKI⁴, Student Member IEEE

ABSTRACT Identifying graph topologies as well as processes evolving over graphs emerge in various applications including transportation, brain, social, and sensor networks. In some of these, the graph structure learning, user activity, transportation, communication, and dynamically interacting nodes are important. In this paper, we propose a graph learning and topology identification framework that accounts for the nonlinear and dynamic dependence of the graph structure learning. We propose a graph learning and topology identification framework that accounts for the nonlinear and dynamic dependence of the graph structure learning. We propose a graph learning and topology identification framework that accounts for the nonlinear and dynamic dependence of the graph structure learning.

INDEX TERMS network-based models, network topology inference, nonlinear learning, network structure

1. INTRODUCTION

The science of networks and structural interactions has recently emerged as a major outlet for understanding the behavior of complex systems [24], [25], [26], [24]. Such systems are especially abundant in graphs, and can be seen in many real-world scenarios. For example, brain networks are used to understand the underlying structure of the brain, and social networks are used to understand the underlying structure of social interactions. In this paper, we propose a graph learning and topology identification framework that accounts for the nonlinear and dynamic dependence of the graph structure learning. We propose a graph learning and topology identification framework that accounts for the nonlinear and dynamic dependence of the graph structure learning.

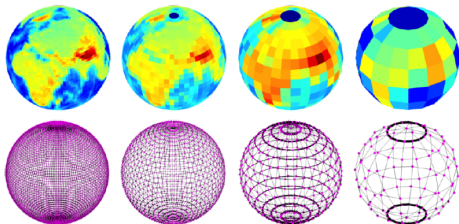
- ▶ IEEE Trans. on Signal and Information Processing over Networks
- ▶ Forthcoming issue on **Network Topology Inference** (Jan. 2020)

Concluding remarks

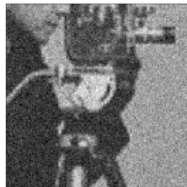
- ▶ **Network science** and big data pose new challenges
 - ⇒ **GSP** can contribute to **address** some of those challenges
 - ⇒ Well suited for **network (diffusion) processes**
- ▶ **GSP pillars**: graph-shift operator, filters and Fourier transform
- ▶ **GSP tools** can be applied **to solve practical problems**
 - ⇒ Signal representation and compression
 - ⇒ Sampling, interpolation (**network control**)
 - ⇒ Source localization on graphs (**fake news, epileptic seizures**)
 - ⇒ Network topology inference
 - ⇒ Geometric deep learning and graph CNNs

Application domains

Visualization / Compression

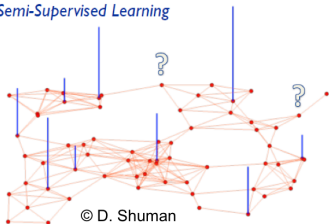


Earth data source: Frederik Simons

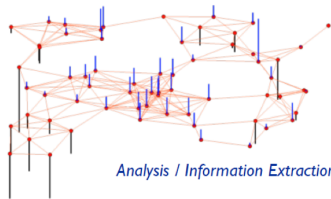


Denoising

Semi-Supervised Learning



© D. Shuman

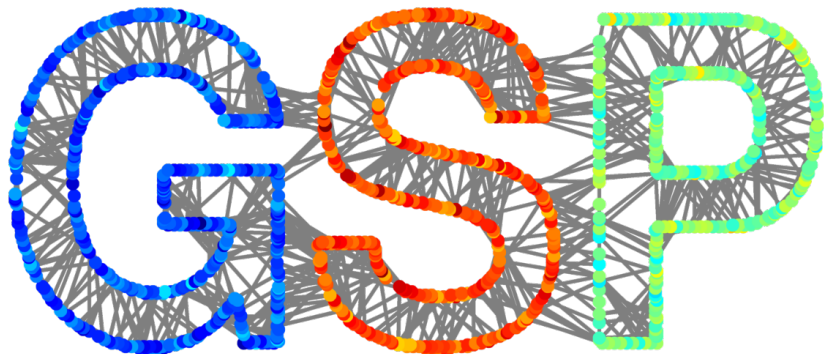


Analysis / Information Extraction

Envisioned application domains

- ▶ Gene regulatory and protein interaction networks
- ▶ Online social media
- ▶ Smart infrastructure networks, IoT
- ▶ Economics, finance, social sciences
- ▶ Neuroimaging data analysis
 - ⇒ Extensive literature on brain network analysis
 - ⇒ Classifying neural disorders, predicting learning ability
 - ⇒ Analyzed networks because they could not study signals
 - ⇒ **GSP**: Integration of structural and functional perspectives

See also [arXiv:1710.01135v3](https://arxiv.org/abs/1710.01135v3) [eess.IV]



- ▶ PyGSP is a Python package to ease SP on graphs. **Free software**

Available from <https://github.com/epfl-lts2/pygsp>