

Graph Signal Processing: Foundational Advances For Learning From Network Data

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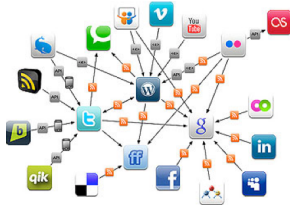
Collaborators: R. Shafipour, S. Segarra, A. G. Marques, and A. Ribeiro

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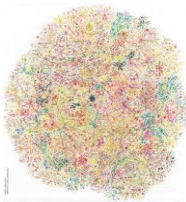
Rochester, NY, October 4, 2019

Network Science analytics

Online social media



Internet



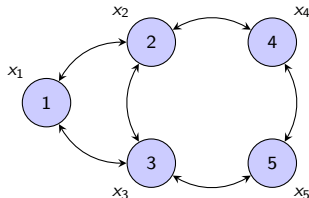
Clean energy and grid analytics



- ▶ **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)

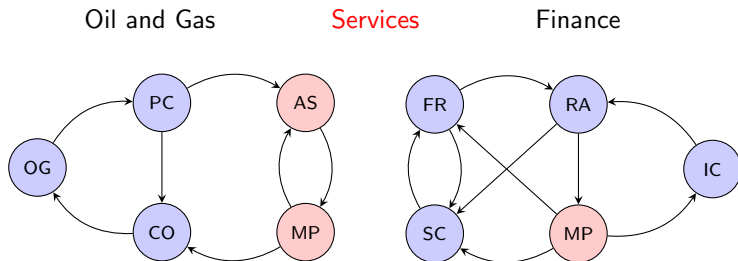
- ▶ Graph G with adjacency matrix $\mathbf{A} \in \mathbb{R}^{N \times N}$
 $\Rightarrow A_{ij}$ = proximity between i and j
- ▶ Define a signal $\mathbf{x} \in \mathbb{R}^N$ on top of the graph
 $\Rightarrow x_i$ = signal value at node i



- ▶ 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

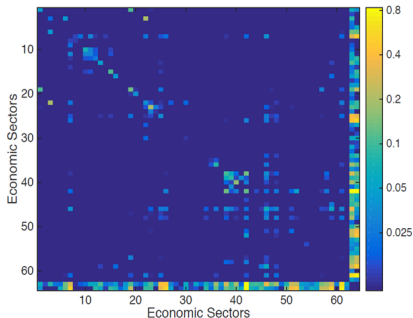
- ▶ Bureau of Economic Analysis of the U.S. Department of Commerce
 - ▶ A_{ij} = Output of sector i that becomes input to sector j (62 sectors)



- ▶ 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

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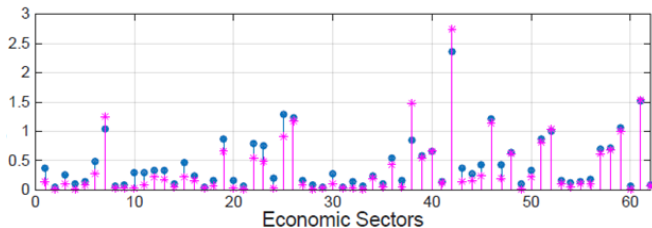


- ▶ A few sectors have widespread strong influence (services, finance, energy)
- ▶ Some sectors have strong indirect influences (oil)
- ▶ The heavy last row is final consumption

- ▶ This is an interesting network \Rightarrow Signals on this graph are as well

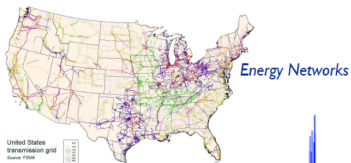
Disaggregated GDP of the United States

- ▶ Signal \mathbf{x} = output per sector = disaggregated GDP
 - ⇒ Network structure used to, e.g., reduce GDP estimation noise

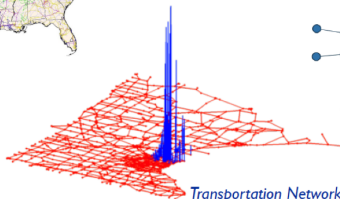
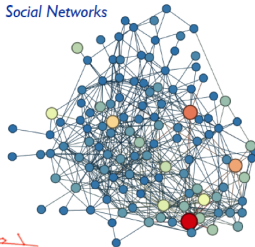


- ▶ Signal is **as interesting as the network itself**. Arguably more
 - ▶ Same is true for brain connectivity and fMRI brain signals, ...
 - ▶ Gene regulatory networks and gene expression levels, ...
 - ▶ Online social networks and information cascades, ...

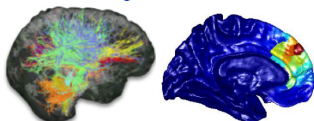
Graph signals are ubiquitous



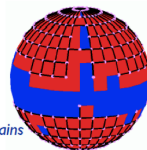
Social Networks



Biological Networks



Irregular Data Domains



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Importance of signal structure in time

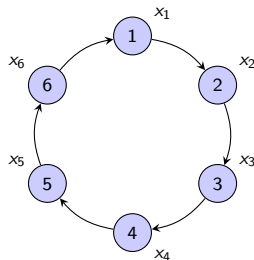
- ▶ Signal and Information Processing **is about exploiting signal structure**

- ▶ 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 $\mathbf{C}_x = \mathbb{E}[\mathbf{x}\mathbf{x}^H]$

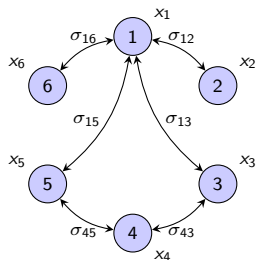
⇒ Eigenvector decomposition $\mathbf{C}_x = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$

- ▶ 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}**

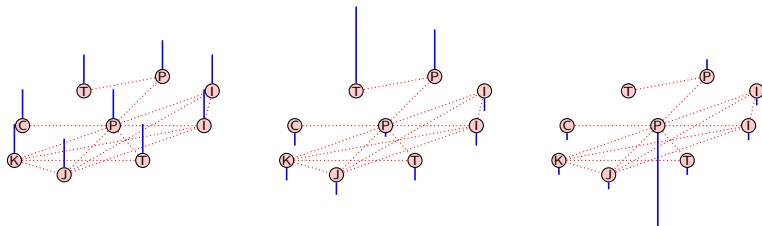
Frequency modes of the Laplacian

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

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

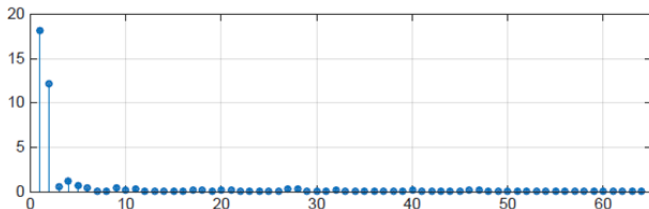
⇒ Smoothness measure on the graph G (Dirichlet energy)

- 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?

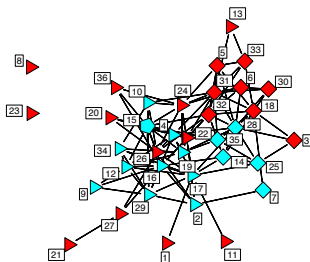
- ▶ Particularized to cyclic graphs \Rightarrow GFT \equiv Fourier transform
- ▶ Also for covariance graphs \Rightarrow GFT \equiv PCA transform
- ▶ But really, this is an **empirical question**. GFT of disaggregated GDP



- ▶ 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

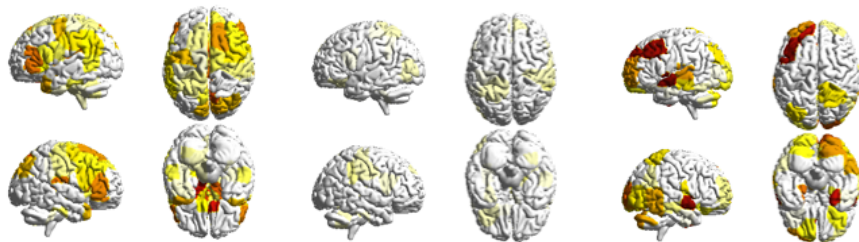
- ▶ Working relationships among lawyers [Lazega'01]
 - ▶ **Graph:** 36 partners, edges indicate partners worked together



- ▶ **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

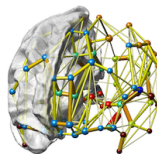
- ▶ GFT of brain signals during a **visual-motor learning task** [Huang et al'16]
 - ⇒ Decomposed into low, medium and high frequency components



- ▶ 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

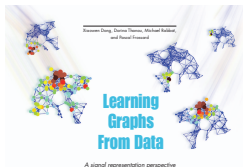
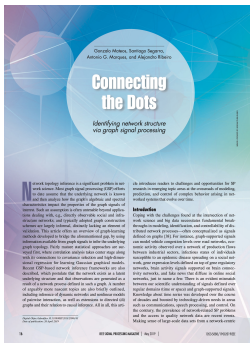
Learning graphs from data

- ▶ **Learning graphs** from nodal observations
- ▶ Key in neuroscience
 - ⇒ Functional network from fMRI signals
- ▶ Most GSP works: how known graph **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 [Pascdeloup 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 dependencies.

By GONZALO B. MATEOS¹, Fellow IEEE, SANTIAGO SEGARRA, Student Member IEEE, and ANTONIO G. MARQUES¹, Student Member IEEE

ABSTRACT Identifying graph topologies as well as processes making use of graph signals in various applications including gene-protein data, social, and neural networks, is seen as a new, key graph-signal learning task. Various topological and dynamical dependencies are captured by graph representations, regularization, and dimensionality reduction. Identifying graph topologies as well as processes making use of graph signals is seen as a new, key graph-signal learning task. Various topological and dynamical dependencies are captured by graph representations, regularization, and dimensionality reduction.

INDEX TERMS Network models, network learning, nonlinear, nonlinear, making use of graph signals.

I. INTRODUCTION

The science of networks and networked information has recently emerged as a major subject for understanding the behavior of complex systems [24], [25], [26]. Such systems are typically described by graphs, that is, by a set of nodes and edges, where nodes represent the main units or elements. For example, human contacts are the nodes in a social network, and the edges represent the connections between them. Similarly, in a neural network, the nodes represent the neurons, and the edges represent the connections between them.

Graphs can be used to model a wide variety of systems, from social networks to biological networks, from communication networks to transportation networks, and from financial networks to power grids. Graphs can be used to model a wide variety of systems, from social networks to biological networks, from communication networks to transportation networks, and from financial networks to power grids.

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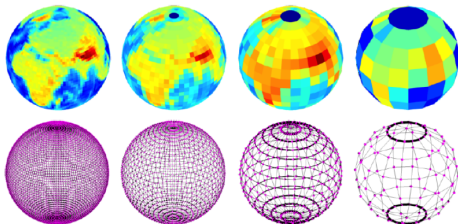
- IEEE Trans. on Signal and Information Processing over Networks
- Forthcoming issue on **Network Topology Inference** (Jan. 2020)

Concluding remarks

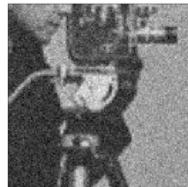
- ▶ Network science and big data pose new challenges
 - ⇒ GSP can contribute to address some of those challenges
 - ⇒ Well suited for network (diffusion) processes
- ▶ GSP pillars: graph-shift operator, filters and Fourier transform
- ▶ GSP tools can be applied to solve practical problems
 - ⇒ Signal 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

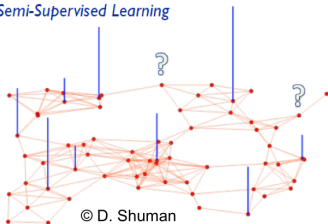


Earth data source: Frederik Simons

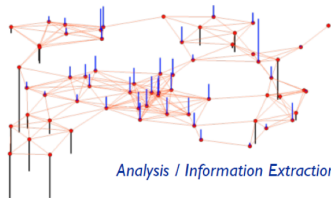


Denoising

Semi-Supervised Learning



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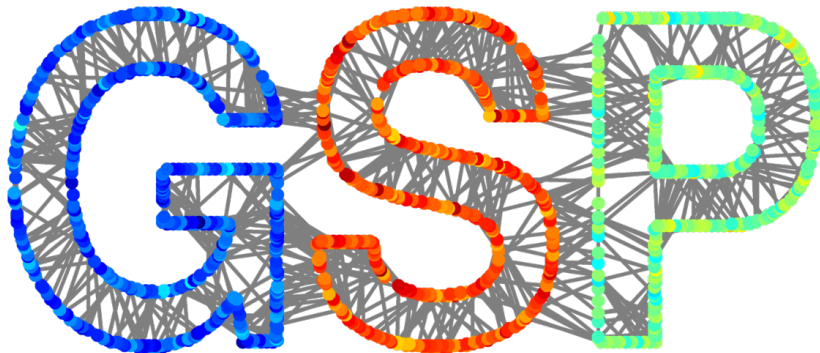
Analysis / Information Extraction

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: Graph Signal Processing in Python



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

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