

Graph Signal Processing: Fundamentals and Applications to Diffusion Processes

Antonio G. Marques[†], Santiago Segarra[‡], Alejandro Ribeiro^{*}

[†]King Juan Carlos University

[‡]Massachusetts Institute of Technology

^{*}University of Pennsylvania

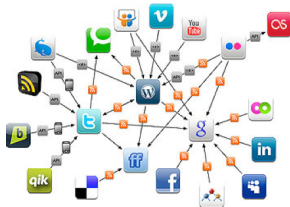
antonio.garcia.marques@urjc.es

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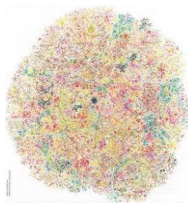
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Budapest, Hungary - August 29, 2016

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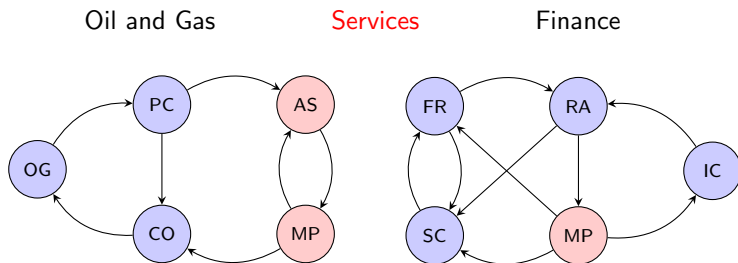


Clean energy and grid analytics



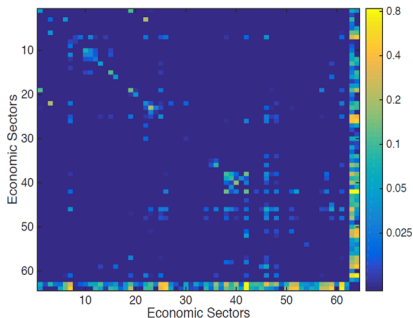
- ▶ **Desiderata:** Process, analyze and learn from **network data** [Kolaczyk'09]
- ▶ **Network as graph** $G = (\mathcal{V}, \mathcal{E}, W)$: encode pairwise relationships
- ▶ Interest here not in G itself, but in **data** associated with **nodes** in \mathcal{V}
⇒ Object of study is a **graph signal** \mathbf{x}
- ▶ **Q:** Graph signals common and interesting as networks are?

- ▶ Bureau of Economic Analysis of the U.S. Department of Commerce
- ▶ \mathcal{E} = Output of sector i is an input to sector j (62 sectors in \mathcal{V})



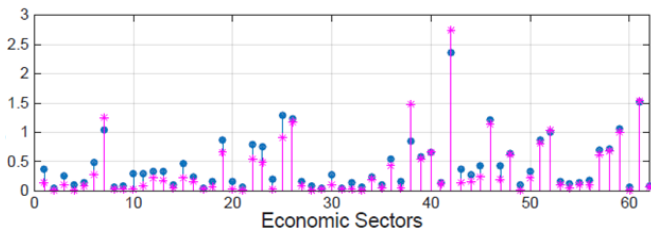
- ▶ Oil extraction (OG), Petroleum and coal products (PC), Construction (CO)
- ▶ Administrative services (AS), **Professional services (MP)**
- ▶ Credit intermediation (FR), Securities (SC), Real state (RA), Insurance (IC)
- ▶ Only interactions stronger than a threshold are shown

- ▶ Bureau of Economic Analysis of the U.S. Department of Commerce
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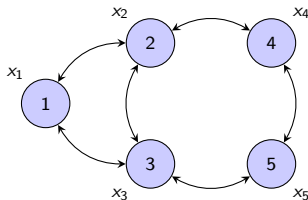
- ▶ A few sectors have widespread strong influence (services, finance, energy)
 - ▶ Some sectors have strong indirect influences (oil)
 - ▶ The heavy last row is final consumption
- ▶ This is an interesting network \Rightarrow Signals on this graph are as well

- ▶ Signal 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 on brain connectivity and fMRI brain signals, ...
 - ▶ Gene regulatory networks and gene expression levels, ...
 - ▶ Online social networks and information cascades, ...
 - ▶ Alignment of customer preferences and product ratings, ...

- ▶ **Graph SP**: broaden classical SP to graph signals [Shuman et al.'13]
⇒ **Our view**: **GSP** well suited to study network (diffusion) processes



- ▶ **As.:** Signal properties related to **topology** of G (locality, smoothness)
⇒ Algorithms that fruitfully **leverage this relational structure**
- ▶ **Q:** Why do we expect the graph structure to be useful in processing \mathbf{x} ?

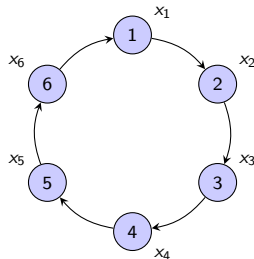
- ▶ Signal and Information Processing **is about exploiting signal structure**

- ▶ 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**

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

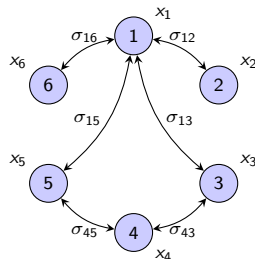
⇒ Eigenvector decomposition $\mathbf{C}_x = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$

- ▶ Covariance matrix \mathbf{C}_x is a graph

⇒ Not a very good graph, but still

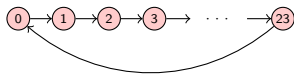
- ▶ Precision matrix \mathbf{C}_x^{-1} a common graph too

⇒ 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?

- ▶ Formally, a graph G (or a network) is a triplet $(\mathcal{V}, \mathcal{E}, W)$
- ▶ $\mathcal{V} = \{1, 2, \dots, N\}$ is a finite set of N nodes or vertices
- ▶ $\mathcal{E} \subseteq \mathcal{V} \times \mathcal{V}$ is a set of edges defined as ordered pairs (n, m)
 - ▶ Write $\mathcal{N}(n) = \{m \in \mathcal{V} : (m, n) \in \mathcal{E}\}$ as the **in-neighbors** of n
- ▶ $W : \mathcal{E} \rightarrow \mathbb{R}$ is a map from the set of edges to scalar values w_{nm}
 - ▶ Represents the **level of relationship** from n to m
 - ▶ Often weights are strictly positive, $W : \mathcal{E} \rightarrow \mathbb{R}_{++}$
- ▶ **Unweighted** graphs $\Rightarrow w_{nm} \in \{0, 1\}$, for all $(n, m) \in \mathcal{E}$
- ▶ **Undirected** graphs $\Rightarrow (n, m) \in \mathcal{E}$ if and only if $(m, n) \in \mathcal{E}$ and $w_{nm} = w_{mn}$, for all $(n, m) \in \mathcal{E}$

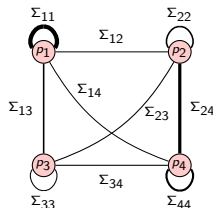
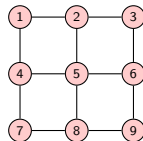


► **Unweighted** and **directed** graphs (e.g., time)

- $\mathcal{V} = \{0, 1, \dots, 23\}$
- $\mathcal{E} = \{(0, 1), (1, 2), \dots, (22, 23), (23, 0)\}$
- $W : (n, m) \mapsto 1$, for all $(n, m) \in \mathcal{E}$

► **Unweighted** and **undirected** graphs (e.g., image)

- $\mathcal{V} = \{1, 2, 3, \dots, 9\}$
- $\mathcal{E} = \{(1, 2), (2, 3), \dots, (8, 9), (1, 4), \dots, (6, 9)\}$
- $W : (n, m) \mapsto 1$, for all $(n, m) \in \mathcal{E}$



► **Weighted** and **undirected** graphs (e.g., covariance)

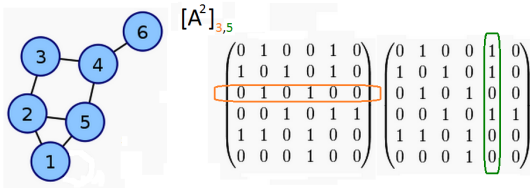
- $\mathcal{V} = \{1, 2, 3, 4\}$
- $\mathcal{E} = \{(1, 1), (1, 2), \dots, (4, 4)\} = \mathcal{V} \times \mathcal{V}$
- $W : (n, m) \mapsto \sigma_{nm} = \sigma_{mn}$, for all (n, m)

- ▶ **Algebraic graph theory**: matrices associated with a graph G
 - ⇒ Adjacency **A** and Laplacian **L** matrices
 - ⇒ **Spectral graph theory**: properties of G using spectrum of **A** or **L**
- ▶ Given $G = (\mathcal{V}, \mathcal{E}, W)$, the **adjacency matrix** **A** $\in \mathbb{R}^{N \times N}$ is

$$A_{nm} = \begin{cases} w_{nm}, & \text{if } (n, m) \in \mathcal{E} \\ 0, & \text{otherwise} \end{cases}$$

- ▶ Matrix representation incorporating all information about G
 - ⇒ For **unweighted** graphs, positive entries represent connected pairs
 - ⇒ For **weighted** graphs, also denote proximities between pairs

- ▶ If G is **unweighted** and **undirected**, the **degree** of node i is $|\mathcal{N}(i)|$
 - ⇒ In **directed** graphs, have **out-degree** and an **in-degree**
- ▶ Using the adjacency matrix in the **undirected** case
 - ⇒ For node i : $\deg(i) = \sum_{j \in \mathcal{N}(i)} A_{ij} = \sum_j A_{ij}$
 - ⇒ For all N nodes: **d** = **A1** → Degree matrix: **D** := diag(**d**)
- ▶ **Q**: Can this be extended to k -hop neighbors? → Powers of **A**
 - ⇒ $[\mathbf{A}^k]_{ij}$ non-zero only if there exists a path of length k from i to j
 - ⇒ Support of \mathbf{A}^k : pairs that can be reached in k hops



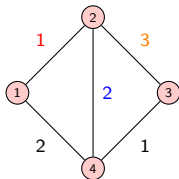
- Given **undirected** G with \mathbf{A} and \mathbf{D} , the Laplacian matrix $\mathbf{L} \in \mathbb{R}^{N \times N}$ is

$$\mathbf{L} = \mathbf{D} - \mathbf{A}$$

\Rightarrow Equivalently, \mathbf{L} can be defined element-wise as

$$L_{ij} = \begin{cases} \deg(i), & \text{if } i = j \\ -w_{ij}, & \text{if } (i, j) \in \mathcal{E} \\ 0, & \text{otherwise} \end{cases}$$

- Normalized Laplacian: $\mathcal{L} = \mathbf{D}^{-1/2} \mathbf{L} \mathbf{D}^{-1/2}$ (we will focus on \mathbf{L})



$$\mathbf{L} = \begin{bmatrix} 3 & -1 & 0 & -2 \\ -1 & 6 & -3 & -2 \\ 0 & -3 & 4 & -1 \\ -2 & -2 & -1 & 5 \end{bmatrix}$$

- ▶ Denote by λ_i and \mathbf{v}_i the eigenvalues and eigenvectors of \mathbf{L}
- ▶ \mathbf{L} is **positive semi-definite**
 - $\Rightarrow \mathbf{x}^T \mathbf{L} \mathbf{x} = \frac{1}{2} \sum_{(i,j) \in \mathcal{E}} w_{ij} (x_i - x_j)^2 \geq 0$, for all \mathbf{x}
 - \Rightarrow All eigenvalues are nonnegative, i.e. $\lambda_i \geq 0$ for all i
- ▶ A constant vector $\mathbf{1}$ is an **eigenvector** of \mathbf{L} with **eigenvalue** 0

$$[\mathbf{L}\mathbf{1}]_i = \sum_{j \in \mathcal{N}(i)} w_{ij} (1 - 1) = 0$$

\Rightarrow Thus, $\lambda_1 = 0$ and $\mathbf{v}_1 = (1/\sqrt{N}) \mathbf{1}$

- ▶ In connected graphs, it holds that $\lambda_i > 0$ for $i = 2, \dots, N$
 - $\Rightarrow \text{Multiplicity}\{\lambda = 0\} = \text{number of connected components}$

Motivation and preliminaries

Part I: Fundamentals

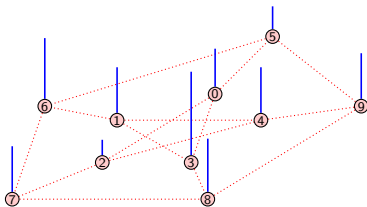
- Graph signals and the shift operator
- Graph Fourier Transform (GFT)
- Graph filters and network processes

Part II: Applications

- Sampling graph signals
- Stationarity of graph processes
- Network topology inference

Concluding remarks

- ▶ Consider graph $G = (\mathcal{V}, \mathcal{E}, W)$. **Graph signals** are mappings $x : \mathcal{V} \rightarrow \mathbb{R}$
 - \Rightarrow Defined on the **vertices** of the **graph** (data tied to nodes)
- Ex:** Opinion profile, buffer congestion levels, neural activity, epidemic
- ▶ May be represented as a vector $\mathbf{x} \in \mathbb{R}^N$
 - $\Rightarrow x_n$ denotes the signal value at the n -th vertex in \mathcal{V}
 - \Rightarrow Implicit ordering of vertices (same as in **A** or **L**)

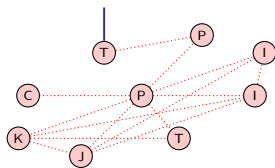


$$\mathbf{x} = \begin{bmatrix} x_0 \\ x_1 \\ x_2 \\ \vdots \\ x_9 \end{bmatrix} = \begin{bmatrix} 0.6 \\ 0.7 \\ 0.3 \\ \vdots \\ 0.7 \end{bmatrix}$$

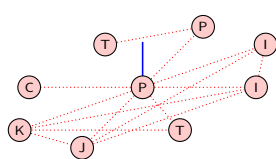
- ▶ Data associated with links of $G \Rightarrow$ Use **line graph** of G

- ▶ Graphs representing **gene-gene interactions**
 - ⇒ Each node denotes a single gene (loosely speaking)
 - ⇒ **Connected** if their coded proteins participate in same metabolism
- ▶ Genetic profiles for each patient can be considered as a **graph signal**
 - ⇒ **Signal on each node** is 1 if mutated and 0 otherwise

$$\mathbf{x}_1 = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$



Sample patient 1 with subtype 1

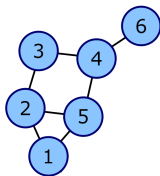


Sample patient 2 with subtype 1

$$\mathbf{x}_2 = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{bmatrix}$$

- ▶ To understand a graph signal, the structure of G must be considered

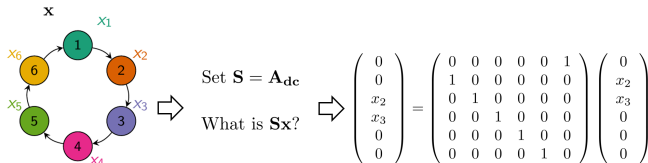
- ▶ To understand and analyze \mathbf{x} , useful to account for G 's structure
- ▶ Associated with G is the **graph-shift** operator $\mathbf{S} \in \mathbb{R}^{N \times N}$
 $\Rightarrow S_{ij} = 0$ for $i \neq j$ and $(i, j) \notin \mathcal{E}$ (captures local structure in G)
- ▶ \mathbf{S} can take **nonzero** values in the **edges** of G or in its **diagonal**



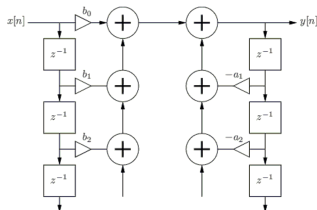
$$\mathbf{S} = \begin{pmatrix} S_{11} & S_{12} & 0 & 0 & S_{15} & 0 \\ S_{21} & S_{22} & S_{23} & 0 & S_{25} & 0 \\ 0 & S_{23} & S_{33} & S_{34} & 0 & 0 \\ 0 & 0 & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & 0 & S_{54} & S_{55} & 0 \\ 0 & 0 & 0 & S_{64} & 0 & S_{66} \end{pmatrix}$$

- ▶ **Ex:** Adjacency \mathbf{A} , degree \mathbf{D} , and Laplacian $\mathbf{L} = \mathbf{D} - \mathbf{A}$ matrices

- **Q:** Why is **S** called shift? **A:** Resemblance to time shifts

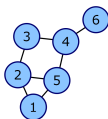


- **S** will be building block for **GSP algorithms** (More soon)
- ⇒ Same is true in the time domain (filters and delay)



\mathbf{S} represents a *linear transformation* that can be *computed locally* at the nodes of the graph. More rigorously, if \mathbf{y} is defined as $\mathbf{y} = \mathbf{S}\mathbf{x}$, then node i can compute y_i if it has access to x_j at $j \in \mathcal{N}(i)$.

- Straightforward because $[\mathbf{S}]_{ij} \neq 0$ only if $i = j$ or $(j, i) \in \mathcal{E}$



$$\Rightarrow \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \\ y_5 \\ y_6 \end{pmatrix} = \begin{pmatrix} S_{11} & S_{12} & 0 & 0 & S_{15} & 0 \\ S_{21} & S_{22} & S_{23} & 0 & S_{25} & 0 \\ 0 & S_{32} & S_{33} & S_{34} & 0 & 0 \\ 0 & 0 & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & 0 & S_{54} & S_{55} & 0 \\ 0 & 0 & 0 & S_{64} & 0 & S_{66} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \\ x_6 \end{pmatrix}$$

- What if $\mathbf{y} = \mathbf{S}^2\mathbf{x}$?

⇒ Like powers of

\mathbf{A} : neighborhoods

⇒ y_i found using values within 2-hops

$$[\mathbf{S}^2]_{3,5} = S_{3,2}S_{2,5} + S_{3,4}S_{4,5}$$

$$\mathbf{S}^2 = \begin{pmatrix} S_{11} & S_{12} & 0 & 0 & S_{15} & 0 \\ S_{21} & S_{22} & S_{23} & 0 & S_{25} & 0 \\ 0 & S_{32} & S_{33} & S_{34} & 0 & 0 \\ 0 & 0 & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & 0 & S_{54} & S_{55} & 0 \\ 0 & 0 & 0 & S_{64} & 0 & S_{66} \end{pmatrix} \begin{pmatrix} S_{11} & S_{12} & 0 & 0 & S_{15} & 0 \\ S_{21} & S_{22} & S_{23} & 0 & S_{25} & 0 \\ 0 & S_{32} & S_{33} & S_{34} & 0 & 0 \\ 0 & 0 & S_{43} & S_{44} & S_{45} & S_{46} \\ S_{51} & S_{52} & 0 & S_{54} & S_{55} & 0 \\ 0 & 0 & 0 & S_{64} & 0 & S_{66} \end{pmatrix}$$

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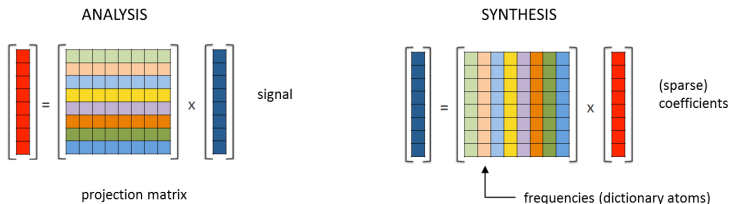
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Concluding remarks

- ▶ Let \mathbf{x} be a temporal signal, its DFT is $\tilde{\mathbf{x}} = \mathbf{F}^H \mathbf{x}$, with $F_{kn} = \frac{1}{\sqrt{N}} e^{+j \frac{2\pi}{N} kn}$
 - ⇒ Equivalent description, provides insights
 - ⇒ Oftentimes, more parsimonious (bandlimited)
 - ⇒ Facilitates the design of SP algorithms: e.g., filters
- ▶ Many other transformations (orthogonal dictionaries) exist



- ▶ **Q:** What transformation is suitable for graph signals?

- ▶ Useful transformation? \Rightarrow \mathbf{S} involved in generation/description of \mathbf{x}
 \Rightarrow Let $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$ be the shift associated with 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

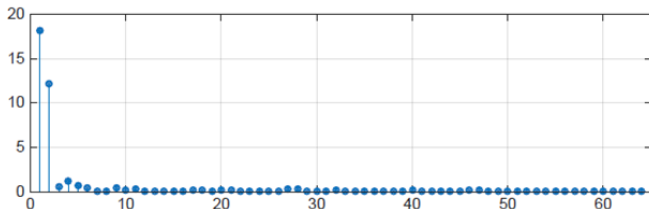
\Rightarrow If \mathbf{S} is normal, then $\mathbf{V}^{-1} = \mathbf{V}^H$ and $\tilde{x}_k = \mathbf{v}_k^H \mathbf{x} = \langle \mathbf{v}_k, \mathbf{x} \rangle$

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

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

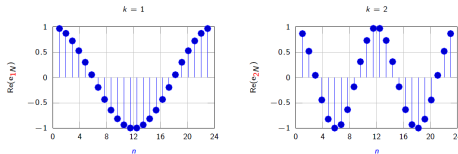
Is this a reasonable transform?

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



- ▶ GFT transform 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

- ▶ Columns of \mathbf{V} are the frequency atoms: $\mathbf{x} = \sum_k \tilde{x}_k \mathbf{v}_k$
- ▶ Q: What about the eigenvalues $\lambda_k = \Lambda_{kk}$
 - \Rightarrow When $\mathbf{S} = \mathbf{A}_{dc}$, we get $\lambda_k = e^{-j\frac{2\pi}{N}k}$
 - $\Rightarrow \lambda_k$ can be viewed as frequencies!!
- ▶ In time, well-defined relation between frequency and variation
 - \Rightarrow Higher $k \Rightarrow$ higher oscillations
 - \Rightarrow Bounds on total-variation: $TV(\mathbf{x}) = \sum_n (x_n - x_{n-1})^2$



- ▶ Q: Does this carry over for graph signals?
 - \Rightarrow No in general, but if $\mathbf{S} = \mathbf{L}$ there are interpretations for λ_k
 - $\Rightarrow \{\lambda_k\}_{k=1}^N$ will be very important when analyzing graph filters

- ▶ Consider a graph G , let \mathbf{x} be a signal on G , and set $\mathbf{S} = \mathbf{L}$
 - $\Rightarrow \mathbf{y} = \mathbf{S}\mathbf{x}$ is now $\mathbf{y} = \mathbf{L}\mathbf{x} \Rightarrow y_i = \sum_{j \in \mathcal{N}(i)} w_{ij}(x_i - x_j)$
 - $\Rightarrow j$ -th term is large if x_j is **very different** from neighboring x_i
 - $\Rightarrow y_i$ **measures difference of x_i relative to its neighborhood**

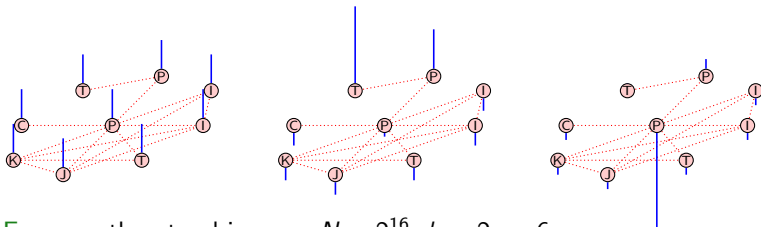
- ▶ We can also define the **quadratic form** $\mathbf{x}^T \mathbf{S} \mathbf{x}$

$$\mathbf{x}^T \mathbf{L} \mathbf{x} = \frac{1}{2} \sum_{(i,j) \in \mathcal{E}} w_{ij} (x_i - x_j)^2$$

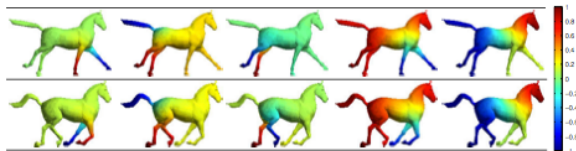
- $\Rightarrow \mathbf{x}^T \mathbf{L} \mathbf{x}$ **quantifies the (aggregated) local variation of signal \mathbf{x}**
- \Rightarrow Natural measure of signal smoothness w.r.t. G

- ▶ **Q:** Interpretation of frequencies $\{\lambda_k\}_{k=1}^N$ when $\mathbf{S} = \mathbf{L}$?
 - \Rightarrow If $\mathbf{x} = \mathbf{v}_k$, we get $\mathbf{x}^T \mathbf{L} \mathbf{x} = \lambda_k \Rightarrow$ local variation of \mathbf{v}_k
 - \Rightarrow Frequencies account for local variation, they can be ordered
 - \Rightarrow Eigenvector associated with eigenvalue 0 is constant

- ▶ Laplacian eigenvalue λ_k accounts for the local variation of \mathbf{v}_k
⇒ Let us plot some of the eigenvectors of \mathbf{L} (also graph signals)
- ▶ Ex: gene network, $N=10$, $k=1$, $k=2$, $k=9$

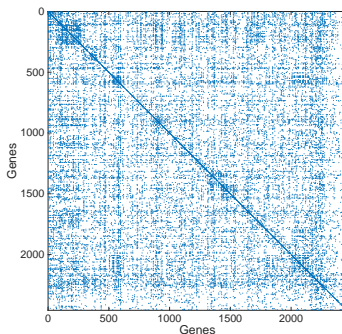


- ▶ Ex: smooth natural images, $N = 2^{16}$, $k = 2, \dots, 6$

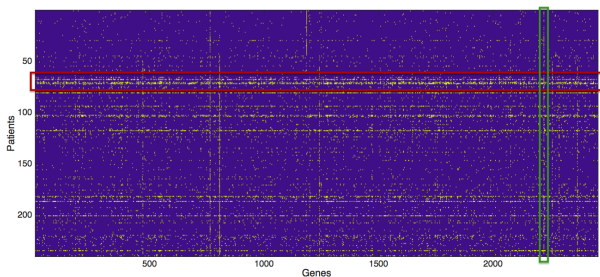


- ▶ Patients diagnosed with same disease exhibit **different behaviors**
- ▶ Each patient has a **genetic profile** describing gene mutations
- ▶ Would be beneficial to infer **phenotypes** from **genotypes**
 - ⇒ Targeted treatments, more suitable suggestions, etc.
- ▶ Traditional approaches consider **different genes** to be independent
 - ⇒ Not ideal, as different genes may **affect same metabolism**
- ▶ Alternatively, consider **genetic network**
 - ⇒ Genetic profiles become **graph signals** on genetic network
 - ⇒ We will see how this consideration improves subtype classification

- ▶ **Undirected** and **unweighted gene-to-gene** interaction graph
 - ▶ 2458 **nodes** are **genes** in human DNA related to breast cancer
 - ▶ An **edge** between two **genes** represents **interaction**
 - ⇒ Coded proteins participate in the **same metabolic process**
- ▶ **Adjacency** matrix of the **gene-interaction** network



- ▶ **Genetic profile** of 240 women with **breast cancer**
 - ⇒ 44 with **serous** subtype and 196 with **endometrioid** subtype
 - ⇒ Patient i has an associated profile $\mathbf{x}_i \in \{0, 1\}^{2458}$
- ▶ **Mutations** are very varied across patients
 - ⇒ Some **patients** present a lot of mutations
 - ⇒ Some **genes** are consistently mutated across patients



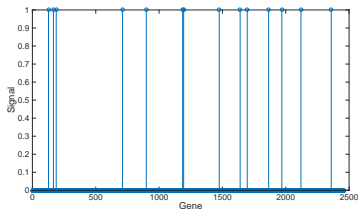
- ▶ **Q:** Can we use **genetic profiles** to **classify** patients across **subtypes**?

- Distance between genetic profiles $\Rightarrow d(i, j) = \|\mathbf{x}_i - \mathbf{x}_j\|_2$
 \Rightarrow N -fold cross-validation error from k -NN classification

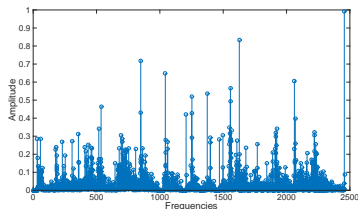
$$k = 3 \Rightarrow 13.3\%, \quad k = 5 \Rightarrow 12.9\%, \quad k = 7 \Rightarrow 14.6\%$$

- Q: Can we do any better using graph signal processing?
- Each genetic profile \mathbf{x}_i is a graph signal on the genetic network
 \Rightarrow Look at the frequency components $\tilde{\mathbf{x}}_i$ using the GFT
 \Rightarrow Use as shift operator \mathbf{S} the Laplacian of the genetic network

Example of signal \mathbf{x}_i



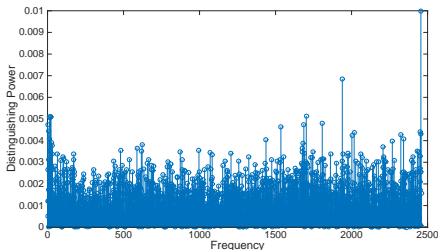
Frequency representation $\tilde{\mathbf{x}}_i$



- Define the **distinguishing power** of frequency \mathbf{v}_k as

$$DP(\mathbf{v}_k) = \left| \frac{\sum_{i:y_i=1} \tilde{\mathbf{x}}_i(k)}{\sum_i \mathbf{1}_{\{y_i=1\}}} - \frac{\sum_{i:y_i=2} \tilde{\mathbf{x}}_i(k)}{\sum_i \mathbf{1}_{\{y_i=2\}}} \right| / \sum_i |\tilde{\mathbf{x}}_i(k)|,$$

- Normalized difference between the mean **GFT** coefficient for \mathbf{v}_k
 \Rightarrow Among **patients** with **serous** and **endometrioid** subtypes
- Distinguishing power** is not equal across **frequencies**

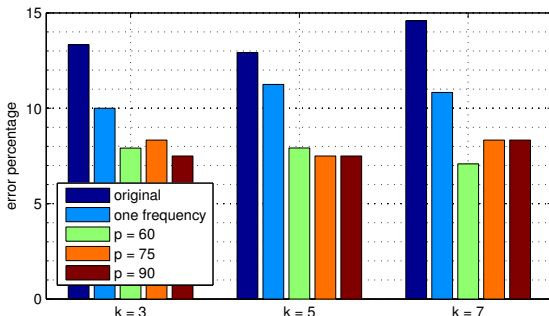


- The distinguishing power defined is one of many proper heuristics

- Keep information in frequencies with higher distinguishing power
⇒ Filter, i.e., multiply $\tilde{\mathbf{x}}_i$ by $\text{diag}(\tilde{\mathbf{h}}^p)$ where

$$[\tilde{\mathbf{h}}^p]_k = \begin{cases} 1, & \text{if } DP(\mathbf{v}_k) \geq p\text{-th percentile of } DP \\ 0, & \text{otherwise} \end{cases}$$

- Then perform inverse GFT to get the graph signal $\hat{\mathbf{x}}_i$



Motivation and preliminaries

Part I: Fundamentals

- Graph signals and the shift operator
- Graph Fourier Transform (GFT)
- Graph filters and network processes

Part II: Applications

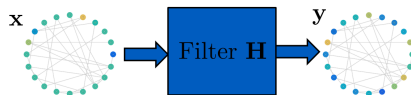
- Sampling graph signals
- Stationarity of graph processes
- Network topology inference

Concluding remarks

- ▶ A graph filter $H : \mathbb{R}^N \rightarrow \mathbb{R}^N$ is a map between graph signals

Focus on linear filters

⇒ map represented by an
 $N \times N$ matrix



DEF1: Polynomial in \mathbf{S} of degree L , with coeff. $\mathbf{h} = [h_0, \dots, h_L]^T$

$$\mathbf{H} := h_0 \mathbf{S}^0 + h_1 \mathbf{S}^1 + \dots + h_L \mathbf{S}^L = \sum_{l=0}^L h_l \mathbf{S}^l \quad [\text{Sandryhaila13}]$$

DEF2: Orthogonal operator in the frequency domain

$$\mathbf{H} := \mathbf{V} \text{diag}(\tilde{\mathbf{h}}) \mathbf{V}^{-1}, \quad \tilde{h}_k = g(\lambda_k)$$

- ▶ With $[\Psi]_{k,l} := \lambda_k^{l-1}$, we have $\tilde{\mathbf{h}} = \Psi \mathbf{h} \Rightarrow$ Defs can be rendered equivalent
⇒ More on this later, now focus on DEF1

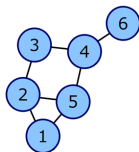
- ▶ DEF1 says $\mathbf{H} = \sum_{l=0}^L h_l \mathbf{S}^l$
- ▶ Suppose \mathbf{H} acts on a graph signal \mathbf{x} to generate $\mathbf{y} = \mathbf{H}\mathbf{x}$
 - ⇒ If we define $\mathbf{x}^{(l)} := \mathbf{S}^l \mathbf{x} = \mathbf{S} \mathbf{x}^{(l-1)}$

$$\mathbf{y} = \sum_{l=0}^L h_l \mathbf{x}^{(l)}$$

\mathbf{y} is a linear combination of successive shifted versions of \mathbf{x}

- ▶ After introducing \mathbf{S} , we stressed that $\mathbf{y} = \mathbf{S}\mathbf{x}$ can be computed locally
 - ⇒ $\mathbf{x}^{(l)}$ can be found locally if $\mathbf{x}^{(l-1)}$ is known
 - ⇒ The output of the filter can be found in L local steps
- ▶ A graph filter represents a linear transformation that
 - ⇒ Accounts for local structure of the graph
 - ⇒ Can be implemented distributedly in L steps
 - ⇒ Only requires info in L -neighborhood [Shuman13, Sandhyala14]

► $\mathbf{x} = [-1, 2, 0, 0, 0, 0]^T$, $\mathbf{h} = [1, 1, 0.5]^T$, $\mathbf{y} = (\sum_{l=0}^L h_l \mathbf{S}) \mathbf{x} = \sum_{l=0}^L h_l \mathbf{x}^{(l)}$



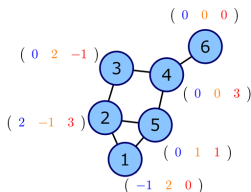
$$\mathbf{S} = \mathbf{A} = \begin{pmatrix} 0 & 1 & 0 & 0 & 1 & 0 \\ 1 & 0 & 1 & 0 & 1 & 0 \\ 0 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 & 0 \end{pmatrix}$$

$$\mathbf{y} = \sum_{l=0}^L h_l \mathbf{S}^l \mathbf{x} = \sum_{l=0}^L h_l \mathbf{x}^{(l)}$$



$$\mathbf{y} = h_0 \mathbf{x}^{(0)} + h_1 \mathbf{x}^{(1)} + h_2 \mathbf{x}^{(2)}$$

Given $\mathbf{x} = [-1, 2, 0, 0, 0, 0]^T$ and $\mathbf{h} = [1, 1, 0.5]^T \Rightarrow$ Find $\{\mathbf{x}^{(0)}, \mathbf{x}^{(1)}, \mathbf{x}^{(2)}\} \Rightarrow$ Find \mathbf{y}



$$\mathbf{x}^{(0)} = \mathbf{x} = \begin{pmatrix} -1 \\ 2 \\ 0 \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad \mathbf{x}^{(1)} = \mathbf{S} \mathbf{x}^{(0)} = \begin{pmatrix} 2 \\ -1 \\ 2 \\ 0 \\ 1 \\ 0 \end{pmatrix} \quad \mathbf{x}^{(2)} = \mathbf{S} \mathbf{x}^{(1)} = \begin{pmatrix} 0 \\ 3 \\ -1 \\ 3 \\ 1 \\ 0 \end{pmatrix}$$

$$\mathbf{y} = 1 \mathbf{x}^{(0)} + 1 \mathbf{x}^{(1)} + 0.5 \mathbf{x}^{(2)} = \begin{pmatrix} 1.0 \\ 2.5 \\ 1.5 \\ 1.5 \\ 1.5 \\ 0.0 \end{pmatrix}$$

- ▶ Recalling that $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^{-1}$, we may write

$$\mathbf{H} = \sum_{l=0}^L h_l \mathbf{S}^l = \sum_{l=0}^L h_l \mathbf{V}\mathbf{\Lambda}^l \mathbf{V}^{-1} = \mathbf{V} \left(\sum_{l=0}^L h_l \mathbf{\Lambda}^l \right) \mathbf{V}^{-1}$$

- ▶ The application $\mathbf{H}\mathbf{x}$ of filter \mathbf{H} to \mathbf{x} can be split into three parts
 - $\Rightarrow \mathbf{V}^{-1}$ takes signal \mathbf{x} to the graph frequency domain $\tilde{\mathbf{x}}$
 - $\Rightarrow \tilde{\mathbf{H}} := \sum_{l=0}^L h_l \mathbf{\Lambda}^l$ modifies the frequency coefficients to obtain $\tilde{\mathbf{y}}$
 - $\Rightarrow \mathbf{V}$ brings the signal $\tilde{\mathbf{y}}$ back to the graph domain \mathbf{y}
- ▶ Since $\tilde{\mathbf{H}}$ is diagonal, define $\tilde{\mathbf{H}} =: \text{diag}(\tilde{\mathbf{h}})$
 - $\Rightarrow \tilde{\mathbf{h}}$ is the frequency response of the filter \mathbf{H}
 - \Rightarrow Output at frequency k depends only on input at frequency k

$$\tilde{y}_k = \tilde{h}_k \tilde{x}_k$$

- Relation between $\tilde{\mathbf{h}}$ and \mathbf{h} in a more friendly manner?
 - ⇒ Since $\tilde{\mathbf{h}} = \text{diag}(\sum_{l=0}^L h_l \boldsymbol{\Lambda}^l)$, we have that $\tilde{h}_k = \sum_{l=0}^L h_l \lambda_k^l$
 - ⇒ Define the Vandermonde matrix Ψ as

$$\Psi := \begin{pmatrix} 1 & \lambda_1 & \dots & \lambda_1^L \\ \vdots & \vdots & & \vdots \\ 1 & \lambda_N & \dots & \lambda_N^L \end{pmatrix}$$

Frequency response of a graph filter

If \mathbf{h} are the coefficients of a graph filter, its frequency response is

$$\tilde{\mathbf{h}} = \Psi \mathbf{h}$$

- Given a desired $\tilde{\mathbf{h}}$, we can find the coefficients \mathbf{h} as

$$\mathbf{h} = \Psi^{-1} \tilde{\mathbf{h}}$$

⇒ Since Ψ is Vandermonde, invertible as long as $\lambda_k \neq \lambda_{k'}$ for $k \neq k'$

- ▶ Since $\mathbf{h} = \Psi^{-1} \tilde{\mathbf{h}} \Rightarrow$ If all $\{\lambda_k\}_{k=1}^N$ distinct, then
 \Rightarrow Any $\tilde{\mathbf{h}}$ can be implemented with at most $L+1 = N$ coefficients
- ▶ Since $\mathbf{h} = \Psi \tilde{\mathbf{h}} \Rightarrow$ If $\lambda_k = \lambda_{k'}$, then
 \Rightarrow The corresponding frequency response will be the same $\tilde{h}_k = \tilde{h}_{k'}$
- ▶ For the particular case when $\mathbf{S} = \mathbf{A}_{dc}$, we have that $\lambda_k = e^{-j\frac{2\pi}{N}(k-1)}$

$$\Psi = \begin{pmatrix} 1 & 1 & \dots & 1 \\ 1 & e^{-j\frac{2\pi(1)(1)}{N}} & \dots & e^{-j\frac{2\pi(1)(N-1)}{N}} \\ \vdots & \vdots & \ddots & \vdots \\ 1 & e^{-j\frac{2\pi(N-1)(1)}{N}} & \dots & e^{-j\frac{2\pi(N-1)(N-1)}{N}} \end{pmatrix} = \mathbf{F}^H$$

\Rightarrow The frequency response is the DFT of the impulse response

$$\tilde{\mathbf{h}} = \mathbf{F}^H \mathbf{h}$$

- ▶ Suppose that we have a signal \mathbf{x} and filter coefficients \mathbf{h}
- ▶ For time signals, it holds that the output \mathbf{y} is

$$\tilde{\mathbf{y}} = \text{diag}(\mathbf{F}^H \mathbf{h}) \mathbf{F}^H \mathbf{x}$$

- ▶ For graph signals, the output \mathbf{y} in the frequency domain is

$$\tilde{\mathbf{y}} = \text{diag}(\boldsymbol{\Psi} \mathbf{h}) \mathbf{V}^{-1} \mathbf{x}$$

- ▶ The **GFT for filters** is different from the **GFT for signals**
 - ⇒ Symmetry is lost, but both depend on spectrum of \mathbf{S}
 - ⇒ Many of the properties are not true for graphs
 - ⇒ Several options to generalize operations

- ▶ Suppose that our goal is to find \mathbf{h} given \mathbf{x} and \mathbf{y}
 - ⇒ Using the previous expressions

$$\mathbf{h} = \Psi^{-1} \text{diag}^{-1}(\mathbf{V}^{-1}\mathbf{x}) \mathbf{V}^{-1}\mathbf{y}$$

- ▶ In time, if we set $\mathbf{x} = [1, 0, \dots, 0]^T = \mathbf{e}_1$ (i.e., $\tilde{\mathbf{x}} = \mathbf{1}$), we have
 - ⇒ $\mathbf{h} = \mathbf{F} \text{diag}^{-1}(\mathbf{1}) \mathbf{F}^H \mathbf{y} = \mathbf{y} \rightarrow \mathbf{h}$ is the impulse response
- ▶ In the graph domain
- ▶ If we set $\mathbf{x} = \mathbf{e}_i$, then $\mathbf{h} = \Psi^{-1} \text{diag}^{-1}(\tilde{\mathbf{e}}_i) \mathbf{V}^{-1}\mathbf{y}$, where
 - ⇒ $\tilde{\mathbf{e}}_i := \mathbf{V}^{-1}\mathbf{e}_i \equiv$ how strongly node i expresses each of the freqs.
 - ⇒ Problem if $\tilde{\mathbf{e}}_i$ has zero entries
- ▶ Alternatively we can get $\tilde{\mathbf{x}} = \mathbf{1}$ by setting $\mathbf{x} = \mathbf{V}\mathbf{1}$ and then
 - ⇒ $\mathbf{h} = \Psi^{-1} \text{diag}^{-1}(\tilde{\mathbf{x}}) \mathbf{V}^{-1}\mathbf{y} = \Psi^{-1} \mathbf{V}^{-1}\mathbf{y}$

- Frequency or space?

$$\mathbf{y} = \mathbf{V} \text{diag}(\tilde{\mathbf{h}}) \mathbf{V}^{-1} \mathbf{x} \quad \text{vs.} \quad \mathbf{y} = \sum_{l=0}^L h_l \mathbf{S}^l \mathbf{x}$$

- In space: leverage the fact that $\mathbf{S}\mathbf{x}$ can be computed locally
 - ⇒ Signal \mathbf{x} is percolated L times to find $\{\mathbf{x}^{(l)}\}_{l=0}^L$
 - ⇒ Every node finds its own y_i by computing $\sum_{l=0}^L h_l [\mathbf{x}^{(l)}]_i$
- Frequency implementation useful for processing if, e.g.,
 - ⇒ Filter bandlimited and eigenvectors easy to find
 - ⇒ Low complexity [Anis16, Tremblay16]
- Space definition useful for modeling
 - ⇒ Diffusion, percolation, opinion formation, ... (more on this soon)
- More on filter design
 - ⇒ Chebyshev polyn. [Shuman12]; AR-MA [Isufi-Leus15]; Node-var. [Segarra15]; Time-var. [Isufi-Leus16]; Median filters [Segarra16]

- Consider a **linear** dynamics of the form

$$\mathbf{x}_t - \mathbf{x}_{t-1} = \alpha \mathbf{J} \mathbf{x}_{t-1} \Rightarrow \mathbf{x}_t = (\mathbf{I} - \alpha \mathbf{J}) \mathbf{x}_{t-1}$$

- If \mathbf{x} is **network process** $\Rightarrow [\mathbf{x}_t]_i$ depends only on $[\mathbf{x}_{t-1}]_j, j \in \mathcal{N}(i)$



$$[\mathbf{S}]_{ij} = [\mathbf{J}]_{ij} \Rightarrow \mathbf{x}_t = (\mathbf{I} - \alpha \mathbf{S}) \mathbf{x}_{t-1} \Rightarrow \mathbf{x}_t = (\mathbf{I} - \alpha \mathbf{S})^t \mathbf{x}_0$$

$$\Rightarrow \mathbf{x}_t = \mathbf{H} \mathbf{x}_0, \text{ with } \mathbf{H} \text{ a polynomial of } \mathbf{S} \Rightarrow \text{linear graph filter}$$

- If the system has **memory** \Rightarrow output weighted sum of previous exchanges (opinion dynamics) \Rightarrow still a **polynomial of \mathbf{S}**

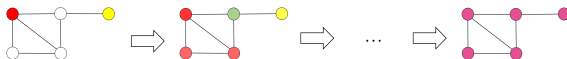
$$\mathbf{y} = \sum_{t=0}^T \beta^t \mathbf{x}_t \Rightarrow \mathbf{y} = \sum_{t=0}^T (\beta \mathbf{I} - \beta \alpha \mathbf{S})^t \mathbf{x}_0$$

- Everything holds true if α_t or β_t are time varying

- ▶ Before finite-time dynamics (FIR filters)
- ▶ Consider now a **diffusion dynamics** $\mathbf{x}_t = \alpha \mathbf{S} \mathbf{x}_{t-1} + \mathbf{w}$

$$\mathbf{x}_t = \alpha^t \mathbf{S}^t \mathbf{x}_0 + \sum_{t'=0}^t \alpha^t \mathbf{S}^{t'} \mathbf{w}$$

\Rightarrow When $t \rightarrow \infty$: $\mathbf{x}_\infty = (\mathbf{I} - \alpha \mathbf{S})^{-1} \mathbf{w} \Rightarrow$ **AR graph filter**



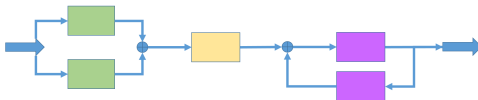
- ▶ Higher orders [Isufi-Leus16]
 - $\Rightarrow M$ **successive** diffusion dynamics \Rightarrow **AR of order M**
 - \Rightarrow Process is the sum of M **parallel** diffusions \Rightarrow **ARMA order M**

$$\mathbf{x}_\infty = \prod_{m=1}^M (\mathbf{I} - \alpha_m \mathbf{S})^{-1} \mathbf{w} \quad \mathbf{x}_\infty = \sum_{m=1}^M (\mathbf{I} - \alpha_m \mathbf{S})^{-1} \mathbf{w}$$

- ▶ Combinations of all the previous are possible

$$\mathbf{x}_t = \mathbf{H}_t^a(\mathbf{S})\mathbf{x}_{t-1} + \mathbf{H}_t^b(\mathbf{S})\mathbf{w} \Rightarrow \mathbf{x}_t = \mathbf{H}_t^A(\mathbf{S})\mathbf{x}_0 + \mathbf{H}_t^B(\mathbf{S})\mathbf{w}$$

$\Rightarrow \mathbf{y} = \mathbf{x}_t$, sequential/parallel application, linear combination

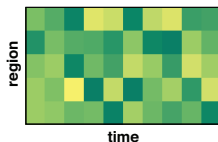


\Rightarrow Expands range of processes that can be modeled via GSP

\Rightarrow Coefficients can change according to some control inputs

- ▶ A number of linear processes can be modeled using graph filters
 - \Rightarrow Theoretical GSP results can be applied to distributed networking
 - \Rightarrow Deconvolution, filtering, system id, ...
 - \Rightarrow Beyond linearity possible too (more at the end of the talk)
- ▶ Links with control theory (of networks and complex systems)
 - \Rightarrow Controllability, observability

- ▶ Why do some people **learn faster** than others?
⇒ Can we answer this by looking at their **brain activity**?
- ▶ **Brain activity** during **learning** of a motor skill in **112 cortical regions**
⇒ **fMRI** while learning a piano pattern for **20 individuals**
- ▶ Pattern is repeated, reducing the time needed for execution
⇒ **Learning** rate = rate of **decrease in execution time**
- ▶ Define a **functional brain graph**
⇒ Based on **correlated** activity
- ▶ **fMRI** outputs a **series of graph signals**
⇒ $\mathbf{x}(t) \in \mathbb{R}^{112}$ describing brain states
- ▶ Does **brain state variability** correlate with **learning**?



- ▶ We propose **three** different **measures** capturing different time scales
⇒ Changes in **micro**, **meso**, and **macro** scales
- ▶ **Micro**: **instantaneous changes** higher than a threshold α

$$m_1(\mathbf{x}) = \sum_{t=1}^T \mathbf{1} \left\{ \frac{\|\mathbf{x}(t) - \mathbf{x}(t-1)\|_2}{\|\mathbf{x}(t)\|_2} > \alpha \right\}$$

- ▶ **Meso**: Cluster brain states and count the **changes in clusters**

$$m_2(\mathbf{x}) = \sum_{t=1}^T \mathbf{1} \{ \mathbf{c}(t) \neq \mathbf{c}(t-1) \}$$

⇒ where $\mathbf{c}(t)$ is the cluster to which $\mathbf{x}(t)$ belongs.

- ▶ **Macro**: **Sample entropy**. Measure of complexity of time series

$$m_3(\mathbf{x}) = -\log \left(\frac{\sum_t \sum_{s \neq t} \mathbf{1} \{ \|\bar{\mathbf{x}}_3(t) - \bar{\mathbf{x}}_3(s)\|_\infty > \alpha \}}{\sum_t \sum_{s \neq t} \mathbf{1} \{ \|\bar{\mathbf{x}}_2(t) - \bar{\mathbf{x}}_2(s)\|_\infty > \alpha \}} \right)$$

⇒ Where $\bar{\mathbf{x}}_r(t) = [\mathbf{x}(t), \mathbf{x}(t+1), \dots, \mathbf{x}(t+r-1)]$

- ▶ We **diffuse** each time signal $\mathbf{x}(t)$ across the brain graph

$$\mathbf{x}_{\text{diff}}(t) = (\mathbf{I} + \beta \mathbf{L})^{-1} \mathbf{x}(t)$$

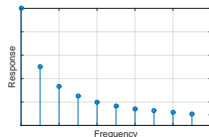
⇒ where **Laplacian** $\mathbf{L} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^{-1}$ and β represents the diffusion rate

- ▶ Analyzing **diffusion** in the frequency domain

$$\tilde{\mathbf{x}}_{\text{diff}}(t) = (\mathbf{I} + \beta \mathbf{\Lambda})^{-1} \mathbf{V}^{-1} \mathbf{x}(t) = \text{diag}(\tilde{\mathbf{h}}) \tilde{\mathbf{x}}(t)$$

⇒ where $\tilde{h}_i = 1/(1 + \beta \lambda_i)$

- ▶ **Diffusion** acts as **low-pass filtering**
- ▶ **High freq.** components are **attenuated**
- ▶ β controls the level of attenuation



- ▶ **Variability** measures consider the **order** of brain signal activity
- ▶ As a **control**, we include in our analysis a **null signal** time series \mathbf{x}_{null}

$$\mathbf{x}_{\text{null}}(t) = \mathbf{x}_{\text{diff}}(\pi_t)$$

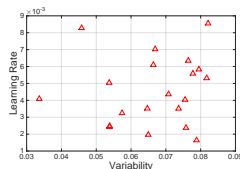
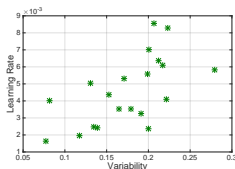
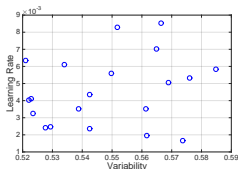
⇒ where π_t is a random **permutation** of the time indices

- ▶ Correlation between **variability** (m_1 , m_2 , and m_3) and **learning**?
- ▶ We consider **three** time series of brain activity
 - ⇒ The **original** fMRI data \mathbf{x}
 - ⇒ The **filtered** data \mathbf{x}_{diff}
 - ⇒ The **null** signal \mathbf{x}_{null}

- Correlation coeff. between **learning rate** and **brain state variability**

	Original	Filtered	Null
m_1	0.211	0.568	0.182
m_2	0.226	0.611	0.174
m_3	0.114	0.382	0.113

- Correlation** is clear when the signal is **filtered**
⇒ Result for **original** signal similar to **null** signal
- Scatter plots for **original**, **filtered**, and **null** signals (m_2 variability)



Motivation and preliminaries

Part I: Fundamentals

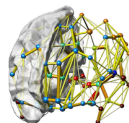
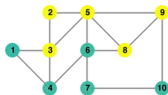
- Graph signals and the shift operator
- Graph Fourier Transform (GFT)
- Graph filters and network processes

Part II: Applications

- Sampling graph signals
- Stationarity of graph processes
- Network topology inference

Concluding remarks

- ▶ Design graph filters to approximate desired network operators
- ▶ Sampling bandlimited graph signals
- ▶ Blind graph filter identification
 - ⇒ Infer diffusion coefficients from observed output
- ▶ Network topology inference
 - ⇒ Infer shift from collection of network diffused signals



- ▶ Many more (not covered, glad to discuss or redirect):
 - ⇒ Statistical GSP, stationarity and spectral estimation
 - ⇒ Filter banks
 - ⇒ Windowing, convolution, duality...
 - ⇒ Nonlinear GSP

Motivation and preliminaries

Part I: Fundamentals

- Graph signals and the shift operator
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Part II: Applications

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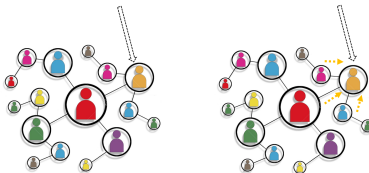
Concluding remarks

- ▶ **Sampling** and **interpolation** are cornerstone problems in **classical SP**
 - ⇒ How recover a signal using only a few observations?
 - ⇒ Need to limit the degrees of freedom: **subspace**, smoothness

- ▶ **Graph signals**: sampling thoroughly investigated
 - ⇒ **Most** assume only **a few values are observed**
 - ⇒ [Anis14, Chen15, Tsitsvero15, Puy15, Wang15]



- ▶ **Alternative approach** [Marques16, Segarra16]
 - ⇒ GSP is well-suited for **distributed networking**
 - ⇒ Incorporate **local graph structure** into the observation model
 - ⇒ Recover signal using distributed **local** graph operators



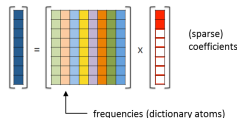
- ▶ **Sampling** is likely to be most important **inverse problem**
 - ⇒ How to find $\mathbf{x} \in \mathbb{R}^N$ using $P < N$ observations?
- ▶ Our focus on **bandlimited** signals, but other models possible

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

⇒ $\mathbf{x} = \sum_{k \in \mathcal{K}} \tilde{x}_k \mathbf{v}_k$, with $|\mathcal{K}| = K < N$

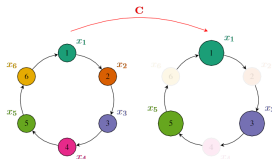
⇒ **S** involved in generation of **x**

⇒ Agnostic to the particular form of **S**

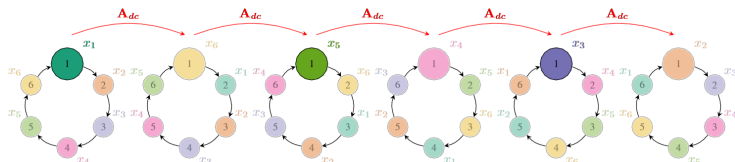


- ▶ Two sampling schemes were introduced in the literature
 - ⇒ **Selection** [Anis14, Chen15, Tsitsvero15, Puy15, Wang15]
 - ⇒ **Aggregation** [Segarra15], [Marques15]
 - ⇒ **Hybrid** scheme combining both ⇒ **Space-shift** sampling
- ▶ More involved, theoretical benefits, practical benefits in distr. setups

- There are **two** ways of interpreting **sampling** of **time signals**
- We can either **freeze** the signal and **sample** values at **different times**



- We can fix a point (**present**) and **sample** the **evolution** of the signal



- Both strategies **coincide** for **time signals** but **not for general graphs**
 \Rightarrow Give rise to **selection** and **aggregation** sampling

- Intuitive generalization to graph signals

$\Rightarrow \mathbf{C} \in \{0, 1\}^{P \times N}$ (matrix P rows of \mathbf{I}_N)

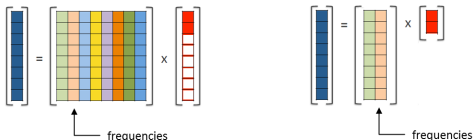
\Rightarrow Sampled signal is $\bar{\mathbf{x}} = \mathbf{C}\mathbf{x}$



- Goal: recover \mathbf{x} based on $\bar{\mathbf{x}}$

\Rightarrow Assume that the support of \mathcal{K} is known (w.l.o.g. $\mathcal{K} = \{k\}_{k=1}^K$)

\Rightarrow Since $\tilde{x}_k = 0$ for $k > K$, define $\tilde{\mathbf{x}}_K := [\tilde{x}_1, \dots, \tilde{x}_K]^T = \mathbf{E}_K^T \tilde{\mathbf{x}}$



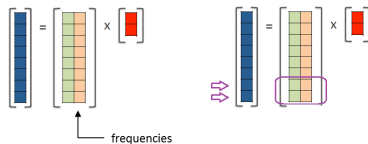
- Approach: use $\bar{\mathbf{x}}$ to find $\tilde{\mathbf{x}}_K$, and then recover \mathbf{x} as

$$\mathbf{x} = \mathbf{V}(\mathbf{E}_K \tilde{\mathbf{x}}_K) = (\mathbf{V}\mathbf{E}_K) \tilde{\mathbf{x}}_K = \mathbf{V}_K \tilde{\mathbf{x}}_K$$

- ▶ Number of samples $P \geq K$

$$\bar{\mathbf{x}} = \mathbf{C}\mathbf{x} = \mathbf{C}\mathbf{V}_K \tilde{\mathbf{x}}_K$$

$\Rightarrow (\mathbf{C}\mathbf{V}_K)$ submatrix of \mathbf{V}



Recovery of selection sampling

If $\text{rank}(\mathbf{C}\mathbf{V}_K) \geq K$, \mathbf{x} can be recovered from the P values in $\bar{\mathbf{x}}$ as

$$\mathbf{x} = \mathbf{V}_K \tilde{\mathbf{x}}_K = \mathbf{V}_K (\mathbf{C}\mathbf{V}_K)^\dagger \bar{\mathbf{x}}$$

- ▶ With $P = K$, hard to check invertibility (by inspection)
 - \Rightarrow Columns of $\mathbf{V}_K (\mathbf{C}\mathbf{V}_K)^{-1}$ are the interpolators
- ▶ In time ($\mathbf{S} = \mathbf{A}_{dc}$), if the samples in \mathbf{C} are equally spaced
 - $\Rightarrow (\mathbf{C}\mathbf{V}_K)$ is Vandermonde (DFT) and $\mathbf{V}_K (\mathbf{C}\mathbf{V}_K)^{-1}$ are sines

- ▶ Idea: incorporating \mathbf{S} to the sampling procedure
⇒ Reduces to classical sampling for time signals
- ▶ Consider shifted (aggregated) signals $\mathbf{y}^{(l)} = \mathbf{S}^l \mathbf{x}$
⇒ $\mathbf{y}^{(l)} = \mathbf{S} \mathbf{y}^{(l-1)} \Rightarrow$ found sequentially with only local exchanges
- ▶ Form $\mathbf{y}_i = [y_i^{(0)}, y_i^{(1)}, \dots, y_i^{(N-1)}]^T$ (obtained locally by node i)



- ▶ The sampled signal is

$$\bar{\mathbf{y}}_i = \mathbf{C} \mathbf{y}_i$$

- ▶ Goal: recover \mathbf{x} based on $\bar{\mathbf{y}}_i$

- ▶ Goal: recover \mathbf{x} based on $\bar{\mathbf{y}}_i \Rightarrow$ Same approach than before
 \Rightarrow Use $\bar{\mathbf{y}}_i$ to find $\tilde{\mathbf{x}}_K$, and then recover \mathbf{x} as $\mathbf{x} = \mathbf{V}_K \tilde{\mathbf{x}}_K$
- ▶ Define $\bar{\mathbf{u}}_i := \mathbf{V}_K^T \mathbf{e}_i$ and recall $\Psi_{kl} = \lambda_k^{l-1}$

Recovery of aggregation sampling

Signal \mathbf{x} can be recovered from the first K samples in $\bar{\mathbf{y}}_i$ as

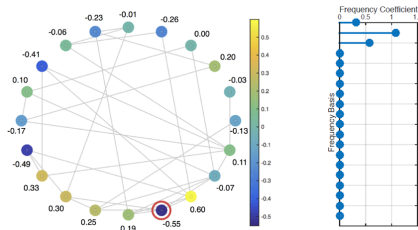
$$\mathbf{x} = \mathbf{V}_K \tilde{\mathbf{x}}_K = \mathbf{V}_K \text{diag}^{-1}(\bar{\mathbf{u}}_i) (\mathbf{C} \Psi^T \mathbf{E}_K)^{-1} \bar{\mathbf{y}}_i$$

provided that $[\bar{\mathbf{u}}_i]_k \neq 0$ and all $\{\lambda_k\}_{k=1}^K$ are distinct.

- ▶ If $\mathbf{C} = \mathbf{E}_K^T$, node i can recover \mathbf{x} with info from $K - 1$ hops!
 - \Rightarrow Node i has to be able to capture frequencies in \mathcal{K}
 - \Rightarrow The frequencies have to distinguishable
- ▶ **Bandlimited signals:** Signals that can be well estimated locally

- In time ($\mathbf{S} = \mathbf{A}_{dc}$), selection and aggregation are equivalent
 \Rightarrow Differences for a more general graph?

- Erdős-Rényi
 $p = 0.2$, $\mathbf{S} = \mathbf{A}$,
 $K = 3$,
 non-smooth



- First 3 observations at node 4: $\mathbf{y}_4 = [0.55, 1.27, 2.94]^T$
 $\Rightarrow [\mathbf{y}_4]_1 = x_4 = -0.55$, $[\mathbf{y}_4]_2 = x_2 + x_3 + x_5 + x_6 + x_7 = 1.27$
 \Rightarrow For this example, any node guarantees recovery
 \Rightarrow Selection sampling fails if, e.g., $\{1, 3, 4\}$

- ▶ Discussion on aggregation sampling
 - ⇒ Observation matrix: **diagonal times Vandermonde**
 - ⇒ Very appropriate in **distributed scenarios**
 - ⇒ Different nodes will lead to different performance (soon)
 - ⇒ Types of signals that are actually bandlimited (role of **S**)
- ▶ Three **extensions**:
 - ⇒ Sampling in the presence of **noise**
 - ⇒ **Unknown** frequency **support**
 - ⇒ Space-shift sampling (**hybrid**)

- ▶ Linear observation model: $\bar{\mathbf{z}}_i = \mathbf{C}\Psi_i\tilde{\mathbf{x}}_K + \mathbf{C}\mathbf{w}_i$ and $\mathbf{x} = \mathbf{V}_K\tilde{\mathbf{x}}_K$
- ▶ BLUE interpolation (Ψ_i either selection or aggregation)

$$\hat{\mathbf{x}}_K^{(i)} = [\Psi_i^H \mathbf{C}^H (\bar{\mathbf{R}}_w^{(i)})^{-1} \mathbf{C} \Psi_i]^{-1} \Psi_i^H \mathbf{C}^H (\bar{\mathbf{R}}_w^{(i)})^{-1} \bar{\mathbf{z}}_i$$

\Rightarrow If $P = K$, then $\hat{\mathbf{x}}^{(i)} = \mathbf{V}_K (\mathbf{C}\Psi_i)^{-1} \bar{\mathbf{z}}_i$

- ▶ Error covariances ($\mathbf{R}_e^{(i)}, \tilde{\mathbf{R}}_e^{(i)}$) in closed form \Rightarrow Noise covariances?
 \Rightarrow Colored, different models: white noise in \mathbf{z}_i , in \mathbf{x} , or in $\tilde{\mathbf{x}}_K$

- ▶ Metric to optimize?

$$\Rightarrow \text{trace}(\mathbf{R}_e^{(i)}), \lambda_{\max}(\mathbf{R}_e^{(i)}), \log \det(\tilde{\mathbf{R}}_e^{(i)}), \left[\text{trace} \left(\tilde{\mathbf{R}}_e^{(i)-1} \right) \right]^{-1}$$

- ▶ Select i and \mathbf{C} to min. error \Rightarrow Depends on metric and noise [Marques16]

- Falls into the class of sparse reconstruction: **observation matrix?**

⇒ Selec. ⇒ **submatrix of unitary** \mathbf{V}_K

⇒ Aggr. ⇒ **Vander. \times diag**

$[\mathbf{u}_i]_k \neq 0$ and $\lambda_k \neq \lambda_{k'} \Rightarrow$ full-spark

$$\begin{bmatrix} \vdots \\ \vdots \\ \vdots \end{bmatrix} = \begin{bmatrix} \text{col 1} & \text{col 2} & \text{col 3} & \text{col 4} & \text{col 5} & \text{col 6} & \text{col 7} & \text{col 8} \end{bmatrix} \times \begin{bmatrix} \text{row 1} \\ \text{row 2} \\ \text{row 3} \\ \text{row 4} \\ \text{row 5} \\ \text{row 6} \\ \text{row 7} \\ \text{row 8} \end{bmatrix}$$

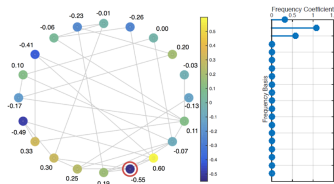
(sparse) coefficients
locations?

- **Joint recovery and support identification** (noiseless)

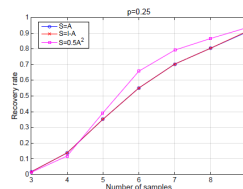
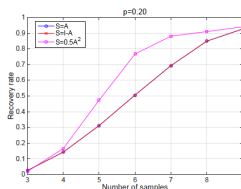
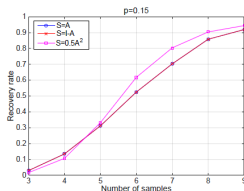
$$\begin{aligned}
 \tilde{\mathbf{x}}^* &:= \arg \min_{\tilde{\mathbf{x}}} \|\tilde{\mathbf{x}}\|_0 \\
 \text{s.t.} \quad & \mathbf{C}\mathbf{y}_i = \mathbf{C}\boldsymbol{\Psi}_i \tilde{\mathbf{x}},
 \end{aligned}$$

- If full spark $\Rightarrow P = 2K$ samples suffice
 - ⇒ Different relaxations are possible
 - ⇒ Conditioning will depend on $\boldsymbol{\Psi}_i$ (e.g., how different $\{\lambda_k\}$ are)
- Noisy case: sampling nodes critical

- Erdős-Rényi
 $p = 0.15, 0.20, 0.25$,
 $K = 3$, non-smooth

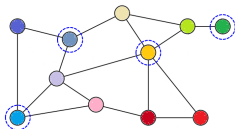


- Three different shifts: \mathbf{A} , $(\mathbf{I} - \mathbf{A})$ and $\frac{1}{2}\mathbf{A}^2$

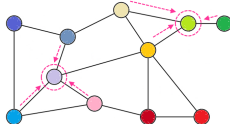


- Space-shift sampling (hybrid) \Rightarrow Multiple nodes and multiple shifts

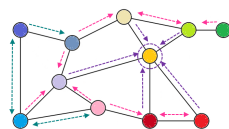
Selection: 4 nodes, 1 sample



Space-shift: 2 nodes, 2 samples



Aggregat.: 1 node, 4 samples

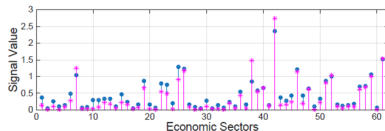
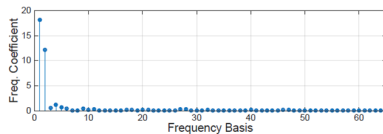
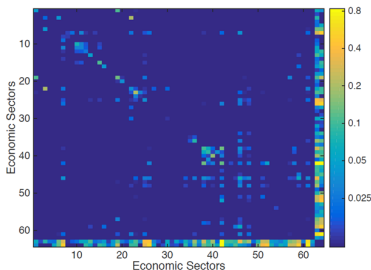


- Section and aggregation sampling as particular cases
- With $\bar{\mathbf{U}} := [\text{diag}(\bar{\mathbf{u}}_1), \dots, \text{diag}(\bar{\mathbf{u}}_N)]^T$, the sampled signal is

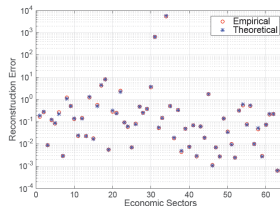
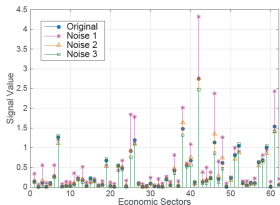
$$\bar{\mathbf{z}} = \mathbf{C} \left(\mathbf{I} \otimes (\boldsymbol{\Psi}^T \mathbf{E}_K) \right) \bar{\mathbf{U}} \tilde{\mathbf{x}}_K + \mathbf{C} \mathbf{w}$$

- As before, BLUE and error covariance in close-form
 - Optimizing sample selection more challenging
 - More structured schemes easier: e.g., message passing
- \Rightarrow Node i knows $y_j^{(l)}$ \Rightarrow node i knows $y_j^{(l')}$ for all $j \in \mathcal{N}_i$ and $l' < l$

- ▶ 62 economic sectors in USA + 2 artificial sectors
 - ⇒ Graph: average flows in 2007-2010, $\mathbf{S} = \mathbf{A}$
 - ⇒ Signal \mathbf{x} : production in 2011
 - ⇒ \mathbf{x} is approximately bandlimited with $K = 4$



- ▶ Setup 1: we add different types of noise
 - ⇒ Error depends on sampling node: better if more connected



- ▶ Setup 2: we try different shift-space strategies

Sampling strategy				Min. error	Median error
$[x]_i$	$[Sx]_i$	$[S^2x]_i$	$[S^3x]_i$.0035	.019
$[x]_i$	$[x]_j$	$[x]_k$	$[x]_l$.0039	4.2
$[Sx]_i$	$[Sx]_j$	$[Sx]_k$	$[Sx]_l$.0035	.030
$[S^2x]_i$	$[S^2x]_j$	$[S^2x]_k$	$[S^2x]_l$.0035	.0055
$[S^3x]_i$	$[S^3x]_j$	$[S^3x]_k$	$[S^3x]_l$.0035	.0040
$[x]_i$	$[Sx]_i$	$[x]_j$	$[Sx]_j$.0035	.039

- ▶ **Beyond bandlimitedness**
 - ⇒ Smooth signals [Chen15]
 - ⇒ Parsimonious in kernelized domain [Romero16]
- ▶ Strategies to **select the sampling nodes**
 - ⇒ Random (sketching) [Varma15]
 - ⇒ Optimal reconstruction [Marques16, Chepuri-Leus16]
 - ⇒ Designed based on posterior task [Gama16]
- ▶ And more...
 - ⇒ **Low-complexity** implementations [Tremblay16, Anis16]
 - ⇒ **Local** implementations [Wang14, Segarra15]
 - ⇒ Unknown spectral decomposition [Anis16]

Motivation and preliminaries

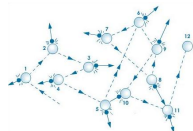
Part I: Fundamentals

- Graph signals and the shift operator
- Graph Fourier Transform (GFT)
- Graph filters and network processes

Part II: Applications

- Sampling graph signals
- Stationarity of graph processes
- Network topology inference

Concluding remarks



- ▶ We frequently encounter **stochastic** processes
- ▶ **Statistical** SP \Rightarrow tools for their understanding
- ▶ **Stationarity** facilitates the analysis of random signals in time
 - \Rightarrow Statistical properties are time-invariant
- ▶ We seek to **extend** the concept of **stationarity** to **graph processes**
 - \Rightarrow Network data and irregular domains motivate this
 - \Rightarrow **Lack of regularity** leads to multiple definitions
- ▶ Classical SSP can be generalized: **spectral estimation, periodograms,...**
 - \Rightarrow **Better understanding** and estimation of **graph processes**
 - \Rightarrow Related works: [Girault 15], [Perraudin 16]

* Segarra, Marques, Leus, Ribeiro, *Stationary Graph Processes: Nonparametric Spectral Estimation*, SAM16

* Marques, Segarra, Leus, Ribeiro, *Stationary Graph Processes and Spectral Estimation*, IEEE TSP (sub.)

- (1) Correlation of stationary discrete time signals is invariant to shifts

$$\mathbf{C}_x := \mathbb{E}[\mathbf{x}\mathbf{x}^H] = \mathbb{E}[\mathbf{x}^H(n-l)_N \mathbf{x}(n-l)_N] = \mathbb{E}[\mathbf{S}^l \mathbf{x} (\mathbf{S}^l \mathbf{x})^H]$$

- (2) Signal is the output of a LTI filter \mathbf{H} excited with white noise \mathbf{w}

$$\mathbf{x} = \mathbf{H}\mathbf{w}, \quad \text{with } \mathbb{E}[\mathbf{w}\mathbf{w}^H] = \mathbf{I}$$

- (3) The covariance matrix \mathbf{C}_x is diagonalized by the Fourier matrix

$$\mathbf{C}_x = \mathbf{F} \text{diag}(\mathbf{p}) \mathbf{F}^H$$

- ▶ The process has a power spectral density $\Rightarrow \mathbf{p} := \text{diag}(\mathbf{F}^H \mathbf{C}_x \mathbf{F})$
- ▶ Each of these definitions can be generalized to graph signals

Definition (shift invariance)

Process \mathbf{x} is weakly stationary with respect to \mathbf{S} if and only if ($b > c$)

$$\mathbb{E}\left[(\mathbf{S}^a \mathbf{x})((\mathbf{S}^H)^b \mathbf{x})^H\right] = \mathbb{E}\left[(\mathbf{S}^{a+c} \mathbf{x})((\mathbf{S}^H)^{b-c} \mathbf{x})^H\right]$$

- ▶ Use a and b shifts as reference. Shift by c forward and backward
⇒ Signal is stationary if these shifts do not alter its covariance
- ▶ It reduces to $\mathbb{E}[\mathbf{x}\mathbf{x}^H] = \mathbb{E}[\mathbf{S}'\mathbf{x}(\mathbf{S}'\mathbf{x})^H]$ when \mathbf{S} is a directed cycle
- ▶ Time shift is orthogonal, $\mathbf{S}^H = \mathbf{S}^{-1}$ ($a = 0$, $b = N$ and $c = I$)
- ▶ Need reference shifts because \mathbf{S} can change energy of the signal

Definition (filtering of white noise)

Process \mathbf{x} is weakly stationary with respect to \mathbf{S} if it can be written as the output of **linear shift invariant filter \mathbf{H}** with white input \mathbf{w}

$$\mathbf{x} = \mathbf{H}\mathbf{w}, \quad \text{with } \mathbb{E} [\mathbf{w}\mathbf{w}^H] = \mathbf{I}$$

- ▶ The filter \mathbf{H} is linear shift invariant if $\Rightarrow \mathbf{H}(\mathbf{S}\mathbf{x}) = \mathbf{S}(\mathbf{H}\mathbf{x})$
- ▶ Equivalently, \mathbf{H} polynomial on the shift operator $\Rightarrow \mathbf{H} = \sum_{l=0}^L h_l \mathbf{S}^l$
- ▶ Filter \mathbf{H} determines color $\Rightarrow \mathbf{C}_{\mathbf{x}} = \mathbb{E} [(\mathbf{H}\mathbf{w})(\mathbf{H}\mathbf{w})^H] = \mathbf{H}\mathbf{H}^H$

Definition (Simultaneous diagonalization)

Process \mathbf{x} is weakly stationary with respect to \mathbf{S} if the **covariance** \mathbf{C}_x and the **shift** \mathbf{S} are **simultaneously diagonalizable**

$$\mathbf{S} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^H \implies \mathbf{C}_x = \mathbf{V} \text{diag}(\mathbf{p}) \mathbf{V}^H$$

- ▶ Equivalent to time definition because \mathbf{F} diagonalizes cycle graph
- ▶ The process has a **power spectral density** $\Rightarrow \mathbf{p} := \text{diag}(\mathbf{V}^H \mathbf{C}_x \mathbf{V})$

- ▶ Have introduced three equally valid definitions of weak stationarity
⇒ They are **different but**, pleasingly, **equivalent**

Proposition

Process \mathbf{x} has shift invariant correlation matrix \Leftrightarrow it is the output of a linear shift invariant filter \Leftrightarrow Covariance jointly diagonalizable with shift

- ▶ Shift and Filtering \Rightarrow How stationary signals look like (local invariance)
- ▶ Simultaneous Diagonalization \Rightarrow A PSD exists $\Rightarrow \mathbf{p} := \text{diag}(\mathbf{V}^H \mathbf{C}_x \mathbf{V})$
 \Rightarrow The PSD collects the eigenvalues of \mathbf{C}_x and is nonnegative

Proposition

*Let \mathbf{x} be stationary in \mathbf{S} and define the process $\tilde{\mathbf{x}} := \mathbf{V}^H \mathbf{x}$. Then, it holds that $\tilde{\mathbf{x}}$ is **uncorrelated** with covariance matrix $\mathbf{C}_{\tilde{\mathbf{x}}} = \mathbb{E} [\tilde{\mathbf{x}} \tilde{\mathbf{x}}^H] = \text{diag}(\mathbf{p})$.*

Example (White noise)

- ▶ White noise \mathbf{w} is stationary in any graph shift $\mathbf{S} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^H$
- ▶ Covariance $\mathbf{C}_w = \sigma^2\mathbf{I}$ simultaneously diagonalizable with all \mathbf{S}

Example (Covariance matrix graphs and Precision matrices)

- ▶ Every process is stationary in the graph defined by its covariance matrix
- ▶ If $\mathbf{S} = \mathbf{C}_x$, shift \mathbf{S} and covariance \mathbf{C}_x diagonalized by same basis
- ▶ Process is also stationary on precision matrix $\mathbf{S} = \mathbf{C}_x^{-1}$

Example (Heat diffusion processes and ARMA processes)

- ▶ Heat diffusion process in a graph $\Rightarrow \mathbf{x} = \alpha_0(\mathbf{I} - \alpha\mathbf{L})^{-1}\mathbf{w}$
- ▶ Stationary in \mathbf{L} since $\alpha_0(\mathbf{I} - \alpha\mathbf{L})^{-1}$ is a polynomial on \mathbf{L}
- ▶ Any autoregressive moving average (ARMA) process on a graph

Example (White noise)

- ▶ Power spectral density $\Rightarrow \mathbf{p} = \text{diag}(\mathbf{V}^H(\sigma^2 \mathbf{I})\mathbf{V}) = \sigma^2 \mathbf{1}$

Example (Covariance matrix graphs and Precision matrices)

- ▶ Power spectral density $\Rightarrow \mathbf{p} = \text{diag}(\mathbf{V}^H(\mathbf{V}\mathbf{\Lambda}\mathbf{V}^H)\mathbf{V}) = \text{diag}(\mathbf{\Lambda})$

Example (Heat diffusion processes and ARMA processes)

- ▶ Power spectral density $\Rightarrow \mathbf{p} = \text{diag}\left[\alpha_0^2 (\mathbf{I} - \alpha \mathbf{\Lambda})^{-2}\right]$

- ▶ Given a process \mathbf{x} , the covariance of $\tilde{\mathbf{x}} = \mathbf{V}^H \mathbf{x}$ is given by

$$\mathbf{C}_{\tilde{\mathbf{x}}} := \mathbb{E} [\tilde{\mathbf{x}} \tilde{\mathbf{x}}^H] = \mathbb{E} [(\mathbf{V}^H \mathbf{x})(\mathbf{V}^H \mathbf{x})^H] = \text{diag}(\mathbf{p})$$

- ▶ **Periodogram** \Rightarrow Given samples $\{\mathbf{x}_r\}_{r=1}^R$, average **GFTs of samples**

$$\hat{\mathbf{p}}_{\text{pg}} := \frac{1}{R} \sum_{r=1}^R |\tilde{\mathbf{x}}_r|^2 = \frac{1}{R} \sum_{r=1}^R |\mathbf{V}^H \mathbf{x}_r|^2$$

- ▶ **Correlogram** \Rightarrow Replace \mathbf{C}_x in PSD definition by **sample covariance**

$$\hat{\mathbf{p}}_{\text{cg}} := \text{diag} \left(\mathbf{V}^H \hat{\mathbf{C}}_x \mathbf{V} \right) := \text{diag} \left[\mathbf{V}^H \left[\frac{1}{R} \sum_{r=1}^R \mathbf{x}_r \mathbf{x}_r^H \right] \mathbf{V} \right]$$

- ▶ **Periodogram** and **correlogram** lead to identical estimates $\hat{\mathbf{p}}_{\text{pg}} = \hat{\mathbf{p}}_{\text{cg}}$

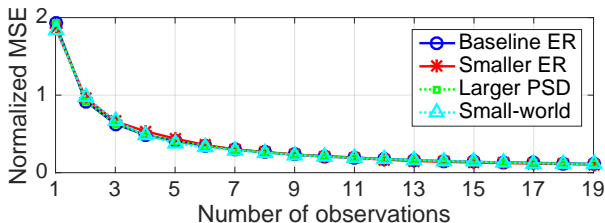
Theorem

If the process \mathbf{x} is Gaussian, periodogram estimates have bias and variance

- ▶ Bias $\Rightarrow \mathbf{b}_{pg} := \mathbb{E}[\hat{\mathbf{p}}_{pg}] - \mathbf{p} = \mathbf{0}$
- ▶ Variance $\Rightarrow \mathbf{\Sigma}_{pg} := \mathbb{E}[(\hat{\mathbf{p}}_{pg} - \mathbf{p})(\hat{\mathbf{p}}_{pg} - \mathbf{p})^H] = \frac{2}{R} \text{diag}^2(\mathbf{p})$
- ▶ The periodogram is unbiased but the variance is not too good
 \Rightarrow Quadratic in \mathbf{p} . Same as time processes
- ▶ Alternative nonparametric methods to reduce variance
 \Rightarrow Average windowed periodogram
 \Rightarrow Filterbanks
 \Rightarrow Bias - variance tradeoff characterized [Marques16, Segarra16]

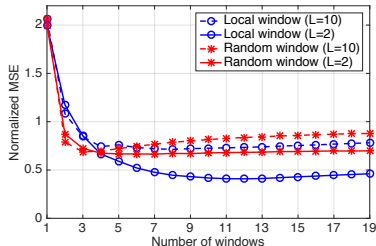
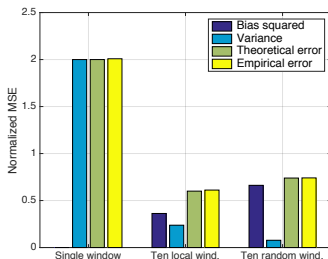
- ▶ PG and CG are examples of **non-parametric** estimators
- ▶ **Parametric ARMA** estimation
 - ⇒ Model $\mathbf{x} = \sum_{l=0}^L h_l \mathbf{S}^l \mathbf{w}$ with \mathbf{w} white
 - ⇒ PSD is $\mathbf{p}_x(\mathbf{h}) = |\boldsymbol{\Psi} \mathbf{h}|^2$
 - ⇒ Given \mathbf{x}_r , compute $\hat{\mathbf{p}}_{pg}$ and find $\hat{\mathbf{h}} = \arg \min_{\mathbf{h}} d(\hat{\mathbf{p}}_{pg}, \mathbf{p}_x(\mathbf{h}))$
 - ⇒ Set $\hat{\mathbf{p}}_{MA} = \mathbf{p}_x(\hat{\mathbf{h}}) = |\boldsymbol{\Psi} \hat{\mathbf{h}}|^2$
 - ⇒ General estimation problem nonconvex
 - ⇒ Particular cases ($\mathbf{S} \succeq \mathbf{0}$ and $\mathbf{h} \succeq \mathbf{0}$) tractable
- ▶ Other **parametric** models (sum of frequency basis) possible too

- ▶ MSE of **periodogram** as a function of the **nr. of observations R**
- ▶ Baseline **ER random graph** ($N = 100$ and $p = 0.05$) and $\mathbf{S} = \mathbf{A}$
- ▶ Observe filtered white Gaussian noise and estimate PSD



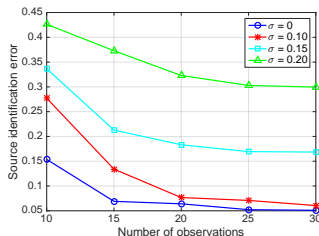
- ▶ Normalized MSE **evolves as $2/R$** as expected
⇒ **Invariant to size, topology, and PSD**
- ▶ Same behavior observed in **non-Gaussian** processes (theory not valid)

- ▶ Performance of **local windows** and **random windows**
- ▶ Block stochastic graph ($N = 100$, 10 communities) and small world
- ▶ Process filters white noise with different number of taps

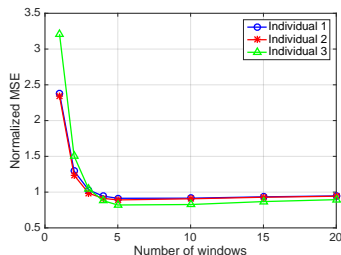
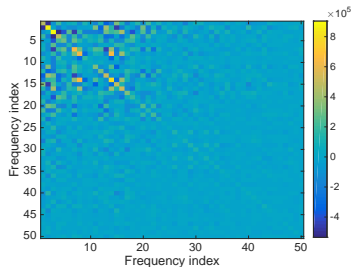


- ▶ The use of windows **introduces bias** but **reduces total error (MSE)**
- ▶ Local windows work better than random windows
⇒ Advantage of **local windows** is larger for **local processes**

- ▶ **Opinion diffusion** in Zachary's karate club network ($N = 34$)
- ▶ Observed **opinion** \mathbf{x} obtained by diffusing sparse white **rumor** \mathbf{w}
- ▶ Given $\{\mathbf{x}_r\}_{r=1}^R$ generated from unknown $\{\mathbf{w}_r\}_{r=1}^R$
⇒ Diffused through filter of unknown nonnegative coefficients β
- ▶ Goal ⇒ **Identify the support** of each rumor \mathbf{w}_r
- ▶ First ⇒ **Estimate** β from Moving Average PSD estimation
- ▶ Second ⇒ Solve R **sparse linear regressions** to recover $\text{supp}(\mathbf{w}_r)$



- ▶ PSD estimation for **spectral signatures** of faces of different people
- ▶ 100 grayscale **face images** $\{\mathbf{x}_i\}_{i=1}^{100} \in \mathbb{R}^{10304}$ (10 images \times 10 people)
- ▶ Consider \mathbf{x}_i as realization graph process that is Stationary on $\hat{\mathbf{C}}_{\mathbf{x}}$
- ▶ Construct $\hat{\mathbf{C}}_{\mathbf{x}}^{(j)} = \mathbf{V}^{(j)} \mathbf{\Lambda}_c^{(j)} \mathbf{V}^{H(j)}$ based on images of person j



- ▶ **Process of person j approximately stationary in $\hat{\mathbf{C}}_{\mathbf{x}}$ (left)**
- ▶ Use **windowed average periodogram** to estimate PSD of new face

- ▶ Extended the notion of **weak stationarity for graph processes**
- ▶ **Three definitions** inspired in stationary time processes
 - ⇒ Shown all of them to be **equivalent**
- ▶ Defined **power spectral density** and studied its estimation
- ▶ Generalized classical **non-parametric estimation** methods
 - ⇒ Periodogram and correlogram where shown to be equivalent
 - ⇒ Windowed average periodogram, filter banks
- ▶ Generalized classical ARMA **parametric estimation** methods
 - ⇒ Particular cases tractable
- ▶ **Extensions**
 - ⇒ Other parametric schemes
 - ⇒ **Space-time** variation

Motivation and preliminaries

Part I: Fundamentals

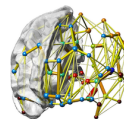
- Graph signals and the shift operator
- Graph Fourier Transform (GFT)
- Graph filters and network processes

Part II: Applications

- Sampling graph signals
- Stationarity of graph processes
- Network topology inference

Concluding remarks

- ▶ Network **topology inference** from nodal observations [Kolaczyk'09]
 - ⇒ Approaches use **Pearson correlations** to construct graphs [Brovelli04]
 - ⇒ Partial correlations and conditional dependence [Friedman08, Karanikolas16]
- ▶ Key in neuroscience [Sporns'10]
 - ⇒ Functional net inferred from activity
- ▶ Most GSP works assume that **S** (hence the graph) is known
 - ⇒ Analyze how the characteristics of **S** affect signals and filters
- ▶ We take the reverse path
 - ⇒ How to use **GSP to infer the graph topology?**
 - ⇒ [Dong15, Mei15, Pavez16, Padeloup16]



†Segarra, Marques, Mateos, Ribeiro, *Network Topology Identification from Spectral Templates*, IEEE SSP16
‡Segarra, Marques, Mateos, Ribeiro, *Network Topology Inference from Spectral Templates*, IEEE TSP (sub.)

- ▶ Given a set of signals $\{\mathbf{x}_r\}_{r=1}^R$ find \mathbf{S}
 - ⇒ We view signals as samples of random graph process \mathbf{x}
 - ⇒ **AS**. \mathbf{x} is **stationary** in \mathbf{S}
- ▶ Equivalent to “ \mathbf{x} is the linear diffusion of a white input”

$$\mathbf{x} = \alpha_0 \prod_{l=1}^{\infty} (\mathbf{I} - \alpha_l \mathbf{S}) \mathbf{w} = \sum_{l=0}^{\infty} \beta_l \mathbf{S}^l \mathbf{w}$$

⇒ Examples: Heat diffusion, structural equation models

$$\mathbf{x} = (\mathbf{I} - \alpha \mathbf{L})^{-1} \mathbf{w} \qquad \mathbf{x} = \mathbf{A} \mathbf{x} + \mathbf{w}$$

- ▶ We say the graph shift **S** **explains the structure of signal x**
- ▶ Key point after assuming **stationarity**: **eigenvectors of the covariance**

- ▶ The covariance matrix of the **stationary** signal $\mathbf{x} = \mathbf{H}\mathbf{w}$ is

$$\mathbf{C}_x = \mathbb{E} [\mathbf{x}\mathbf{x}^H] = \mathbf{H}\mathbb{E} [(\mathbf{w}\mathbf{w}^H)] \mathbf{H}^H = \mathbf{H}\mathbf{H}^H$$

⇒ Since \mathbf{H} is diagonalized by \mathbf{V} , so is the covariance \mathbf{C}_x

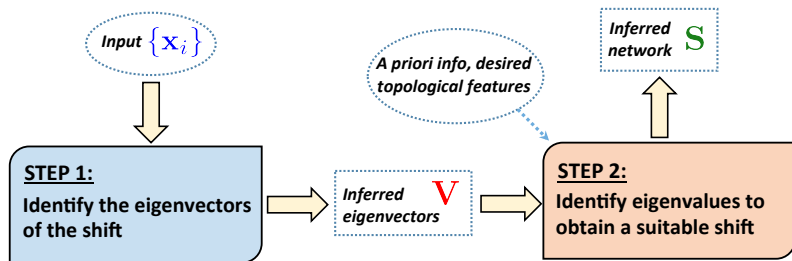
$$\mathbf{C}_x = \mathbf{V} \left| \sum_{l=0}^{L-1} h_l \mathbf{\Lambda}^l \right|^2 \mathbf{V}^H = \mathbf{V} \text{diag}(\mathbf{p}) \mathbf{V}^H$$

- ▶ Any shift with eigenvectors \mathbf{V} can explain \mathbf{x}
 - ⇒ G and its **specific eigenvalues** have been **obscured** by diffusion

Observations

- (a) There are **many shifts** that can explain a signal \mathbf{x}
- (b) Identifying the shift \mathbf{S} is just a matter of **identifying the eigenvalues**
- (c) In **correlation** methods the **eigenvalues** are kept **unchanged**
- (d) In **precision** methods the **eigenvalues** are **inverted**

- We propose a **two-step approach** for graph topology identification



- Beyond diffusion \Rightarrow alternative sources for **spectral templates V**
 \Rightarrow Graph sparsification, network deconvolution,...

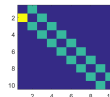
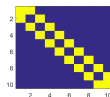
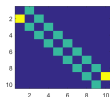
1) Graph sparsification

- ▶ Goal: given \mathbf{S}_f find sparser \mathbf{S} with same eigenvectors
⇒ Find $\mathbf{S}_f = \mathbf{V}_f \mathbf{\Lambda}_f \mathbf{V}_f^H$ and set $\mathbf{V} = \mathbf{V}_f$
⇒ Oftentimes referred to as **network deconvolution** problem

2) Nodal relation assumed by a given transform

- ▶ GSP: decompose $\mathbf{S} = \mathbf{V} \mathbf{\Lambda} \mathbf{V}^H$ and set \mathbf{V}^H as GFT
- ▶ SP: some transforms \mathbf{T} known to work well on specific data
- ▶ Goal: given \mathbf{T} , set $\mathbf{V}^H = \mathbf{T}$ and identify $\mathbf{S} \Rightarrow$ intuition on data relation

DCTs: i-iii



3) Implementation of linear network operators

- ▶ Goal: distributed implementation of **linear operator** \mathbf{B} via graph filter
⇒ Feasible if \mathbf{B} and \mathbf{S} share eigenvectors \Rightarrow Like 1) with $\mathbf{S}_f = \mathbf{B}$

STEP 2: Obtaining the eigenvalues

- ▶ Given \mathbf{V} , there are many possible $\mathbf{S} = \mathbf{V} \text{diag}(\boldsymbol{\lambda}) \mathbf{V}^H$
 - \Rightarrow We can use extra knowledge/assumptions to choose one graph
 - \Rightarrow Of all graphs, select one that is **optimal** in some sense

$$\mathbf{S}^* := \underset{\mathbf{S}, \boldsymbol{\lambda}}{\operatorname{argmin}} f(\mathbf{S}, \boldsymbol{\lambda}) \quad \text{s. to} \quad \mathbf{S} = \sum_{k=1}^N \lambda_k \mathbf{v}_k \mathbf{v}_k^H, \quad \mathbf{S} \in \mathcal{S} \quad (1)$$

- ▶ Set \mathcal{S} contains all admissible scaled **adjacency** matrices

$$\mathcal{S} := \{\mathbf{S} \mid S_{ij} \geq 0, \mathbf{S} \in \mathcal{M}^N, S_{ii} = 0, \sum_j S_{1j} = 1\}$$

- \Rightarrow Can accommodate **Laplacian** matrices as well
- ▶ Problem is convex if we select a convex objective $f(\mathbf{S}, \boldsymbol{\lambda})$
 - \Rightarrow **Minimum energy** ($f(\mathbf{S}) = \|\mathbf{S}\|_F$), **Fast mixing** ($f(\boldsymbol{\lambda}) = -\lambda_2$)

- ▶ The feasibility set in (1) is generally small \Rightarrow Why?
 - \Rightarrow We search over $\lambda \in \mathbb{R}^N$, we have N linear constraints $S_{ii} = 0$
- ▶ This helps in the optimization, to be rigorous
 - \Rightarrow Define $\mathbf{W} := \mathbf{V} \odot \mathbf{V}$ where \odot is the Khatri-Rao product
 - \Rightarrow Denote by \mathcal{D} the index set such that $\text{vec}(\mathbf{S})_{\mathcal{D}} = \text{diag}(\mathbf{S})$

Assume that (1) is feasible, then it holds that $\text{rank}(\mathbf{W}_{\mathcal{D}}) \leq N - 1$.
If $\text{rank}(\mathbf{W}_{\mathcal{D}}) = N - 1$, then the feasible set of (1) is a **singleton**.

- ▶ **Convex feasibility set** \Rightarrow Search for the optimal solution may be easy
- ▶ Simulations will show that $\text{rank}(\mathbf{W}_{\mathcal{D}}) = N - 1$ arises in practice

- ▶ Whenever the feasibility set of (1) is non-trivial
 $\Rightarrow f(\mathbf{S}, \boldsymbol{\lambda})$ determines the features of the recovered graph

Ex: Identify the **sparsest shift** \mathbf{S}_0^* that explains observed signal structure
 \Rightarrow Set the cost $f(\mathbf{S}, \boldsymbol{\lambda}) = \|\mathbf{S}\|_0$

$$\mathbf{S}_0^* = \underset{\mathbf{S}, \boldsymbol{\lambda}}{\operatorname{argmin}} \|\mathbf{S}\|_0 \quad \text{s. to} \quad \mathbf{S} = \sum_{k=1}^N \lambda_k \mathbf{v}_k \mathbf{v}_k^T, \quad \mathbf{S} \in \mathcal{S}$$

- ▶ Problem is not convex, but can **relax to ℓ_1 norm** minimization

$$\mathbf{S}_1^* := \underset{\mathbf{S}, \boldsymbol{\lambda}}{\operatorname{argmin}} \|\mathbf{S}\|_1 \quad \text{s. to} \quad \mathbf{S} = \sum_{k=1}^N \lambda_k \mathbf{v}_k \mathbf{v}_k^H, \quad \mathbf{S} \in \mathcal{S}$$

- ▶ Does the solution \mathbf{S}_1^* coincide with the ℓ_0 solution \mathbf{S}_0^* ?

- ▶ Denoting by \mathbf{m}_i^T the i -th row of $\mathbf{M} := (\mathbf{I} - \mathbf{W}\mathbf{W}^\dagger)_{\mathcal{D}^c}$
 - \Rightarrow Construct $\mathbf{R} := [\mathbf{m}_2 - \mathbf{m}_1, \dots, \mathbf{m}_{N-1} - \mathbf{m}_1, \mathbf{m}_N, \dots, \mathbf{m}_{|\mathcal{D}^c|}]^T$
 - \Rightarrow Denote by \mathcal{K} the indices of the support of $\mathbf{s}_0^* = \text{vec}(\mathbf{S}_0^*)$

\mathbf{S}_1^* and \mathbf{S}_0^* coincide if the two following conditions are satisfied:

- 1) $\text{rank}(\mathbf{R}_{\mathcal{K}}) = |\mathcal{K}|$; and
- 2) There exists a constant $\delta > 0$ such that

$$\psi_{\mathbf{R}} := \|\mathbf{I}_{\mathcal{K}^c}(\delta^{-2}\mathbf{R}\mathbf{R}^T + \mathbf{I}_{\mathcal{K}^c}^T\mathbf{I}_{\mathcal{K}^c})^{-1}\mathbf{I}_{\mathcal{K}}^T\|_{\infty} < 1.$$

- ▶ Cond. 1) ensures uniqueness of solution \mathbf{S}_1^*
- ▶ Cond. 2) guarantees existence of a dual certificate for ℓ_0 optimality

- ▶ We might have access to $\hat{\mathbf{V}}$, a **noisy version** of the spectral templates
 \Rightarrow With $d(\cdot, \cdot)$ denoting a (convex) **distance** between matrices

$$\min_{\{\mathbf{S}, \boldsymbol{\lambda}, \hat{\mathbf{S}}\}} \|\mathbf{S}\|_1 \quad \text{s. to} \quad \hat{\mathbf{S}} = \sum_{k=1}^N \lambda_k \hat{\mathbf{v}}_k \hat{\mathbf{v}}_k^T, \quad \mathbf{S} \in \mathcal{S}, \quad d(\mathbf{S}, \hat{\mathbf{S}}) \leq \epsilon$$

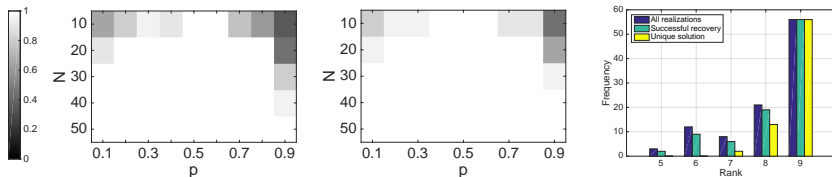
- ▶ Recovery result similar to the noiseless case can be derived
 \Rightarrow Conditions under which we are guaranteed $d(\mathbf{S}^*, \mathbf{S}_0^*) \leq C\epsilon$

- ▶ Partial access to $\mathbf{V} \Rightarrow$ Only K known eigenvectors $[\mathbf{v}_1, \dots, \mathbf{v}_K]$

$$\min_{\{\mathbf{S}, \mathbf{S}_{\bar{K}}, \boldsymbol{\lambda}\}} \|\mathbf{S}\|_1 \quad \text{s. to} \quad \mathbf{S} = \mathbf{S}_{\bar{K}} + \sum_{k=1}^K \lambda_k \mathbf{v}_k \mathbf{v}_k^T, \quad \mathbf{S} \in \mathcal{S}, \quad \mathbf{S}_{\bar{K}} \mathbf{v}_k = \mathbf{0}$$

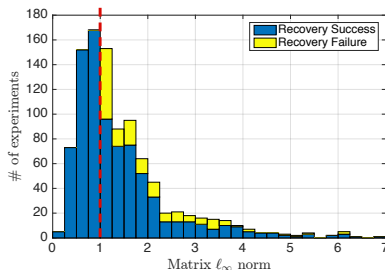
- ▶ Incomplete and noisy scenarios can be combined

- ▶ Erdős-Rényi graphs of varying size $N \in \{10, 20, \dots, 50\}$
 - ⇒ Edge probabilities $p \in \{0.1, 0.2, \dots, 0.9\}$
- ▶ Recovery rates for adjacency (left) and normalized Laplacian (mid)



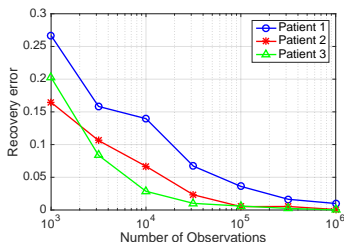
- ▶ Recovery is easier for intermediate values of p
- ▶ Rate of recovery related to the $\text{rank}(\mathbf{W}_D)$ (histogram $N=10, p=0.2$)
 - ⇒ When rank is $N - 1$, recovery is guaranteed
 - ⇒ As rank decreases, there is a detrimental effect on recovery

- ▶ Generate 1000 ER random graphs ($N = 20$, $p = 0.1$) such that
 - ⇒ Feasible set is not a singleton
 - ⇒ Cond. 1) in sparse recovery theorem is satisfied
- ▶ Noiseless case: ℓ_1 norm guarantees recovery as long as $\psi_R < 1$



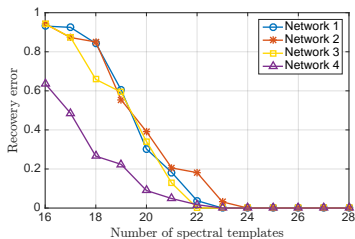
- ▶ Condition is sufficient but **not necessary**
 - ⇒ **Tightest** possible bound on this matrix norm

- Identification of structural brain graphs $N = 66$
- Test recovery for noisy spectral templates $\hat{\mathbf{V}}$
 - ⇒ Obtained from sample covariances of diffused signals



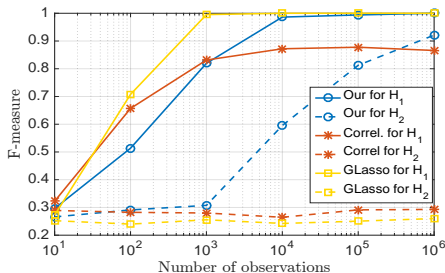
- Recovery error decreases with increasing number of observed signals
 - ⇒ More reliable estimate of the covariance ⇒ Less noisy $\hat{\mathbf{V}}$
- Brain of patient 1 is consistently the hardest to identify
 - ⇒ Robustness for identification in noisy scenarios
- Traditional methods like graphical lasso fail to recover \mathbf{S}

- Identification of multiple social networks $N = 32$
 - ⇒ Defined on the same node set of students from Ljubljana
- Test recovery for **incomplete** spectral templates $\hat{\mathbf{V}} = [\mathbf{v}_1, \dots, \mathbf{v}_K]$
 - ⇒ Obtained from a low-pass diffusion process
 - ⇒ **Repeated** eigenvalues in \mathbf{C}_x introduce **rotation ambiguity** in \mathbf{V}



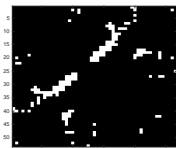
- Recovery error decreases with increasing nr. of **spectral templates**
 - ⇒ Performance improvement is sharp and precipitous

- ▶ Comparison with **graphical lasso** and **sparse correlation** methods
 - ▶ Evaluated on 100 realizations of ER graphs with $N = 20$ and $p = 0.2$

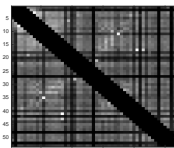


- ▶ Graphical lasso **implicitly assumes a filter** $\mathbf{H}_1 = (\rho \mathbf{I} + \mathbf{S})^{-1/2}$
 - ⇒ For this filter spectral templates work, but not as well (MLE)
- ▶ For **general** diffusion **filters** \mathbf{H}_2 spectral templates still work fine

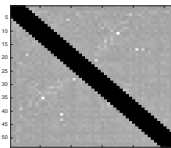
- ▶ Our method can be used to **sparsify a given network**
- ▶ Keep direct and important edges or relations
 - ⇒ **Discard indirect relations** that can be explained by direct ones
- ▶ Use **eigenvectors \hat{V} of given network** as noisy templates
- ▶ Infer **contact between amino-acid residues** in BPT1 BOVIN
 - ⇒ Use mutual information of amino-acid covariation as input



Ground truth



Mutual info.



Network deconv.



Our approach

- ▶ Network deconvolution assumes a specific filter model [Feizi13]
 - ⇒ We achieve better performance by being agnostic to this

- ▶ Network **topology inference** cornerstone problem in Network Science
 - ▶ Most GSP works analyze how **S** affect signals and filters
 - ▶ Here, reverse path: How to use **GSP to infer the graph topology?**
- ▶ Our GSP approach to network **topology inference**
 - ⇒ **Two step** approach: i) Obtain **V**; ii) Estimate **S** given **V**
- ▶ How to obtain the spectral templates **V**
 - ⇒ Based on **covariance of diffused signals**
 - ⇒ Other sources too: net operators, data transforms
- ▶ Infer **S** via **convex optimization**
 - ⇒ Objectives promotes desirable properties
 - ⇒ Constraints encode structure a priori info and structure
 - ⇒ Formulations for **perfect and imperfect templates**
 - ⇒ **Sparse recovery** results for both adjacency and Laplacian

Motivation and preliminaries

Part I: Fundamentals

- Graph signals and the shift operator
- Graph Fourier Transform (GFT)
- Graph filters and network processes

Part II: Applications

- Sampling graph signals
- Stationarity of graph processes
- Network topology inference

Concluding remarks

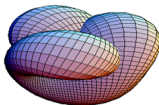
- ▶ Network science and big data pose new challenges
 - ⇒ GSP can contribute to solve some of those challenges
 - ⇒ Well suited for network (diffusion) processes
- ▶ Central elements in GSP: graph-shift operator and Fourier transform
- ▶ Graph filters: operate graph signals
 - ⇒ Polynomials of the shift operator that can be implemented locally
- ▶ Network diffusion/percolations processes via graph filters
 - ⇒ Successive/parallel combination of local linear dynamics
 - ⇒ Possibly time-varying diffusion coefficients
 - ⇒ Accurate to model certain setups
 - ⇒ GSP yields insights on how those processes behave

- **GSP results** can be applied to solve practical problems
 - ⇒ Sampling, interpolation (**network control**)
 - ⇒ Input and system ID (**rumor ID**)
 - ⇒ Shift design (**network topology ID**)

Interpolate a brain signal
from local observations



Compress a signal in
an irregular domain



Localize the
source of a rumor



Smooth an observed
network profile



Predict the evolution of a
network process



Infer the topology where
the signals reside

- ▶ **First step to challenging problems:** social nets, brain signals
- ▶ Motivates **further research:**
 - ⇒ Space-time variation
 - ⇒ Changing topologies
 - ⇒ Nonlinear approaches
 - ⇒ Local, reduced-complexity algorithms
- ▶ **Thanks!**
 - ⇒ If you have questions, feel free to contact me by e-mail antonio.garcia.marques@urjc.es or any of the other authors.

We include a list of our published work in graph signal processing (GSP) categorized by topic. We also include relevant works by other authors. This latter list is not intended to be exhaustive but rather its purpose is to guide the interested reader to pertinent publications in different areas of graph signal processing.

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Blind graph deconvolution

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