Learning Flexible Representations of Stochastic Processes on Graphs

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Introduction

We study filtering of time-varying graph signals on directed (or undirected) graphs in the context of representation learning and graph convolutional networks. Our two primary contributions are an expressive graphical model using Laurent graph-shift operators and a flexible filter design framework using functional calculus.

Modeling Time-Varying Graph Signals

Let $\mathcal{G}$ be a graph with nodes $\mathcal{V} = \{0, \ldots, n-1\}$. Time-varying graph signals are sequences,

$$\mathbf{x} = \left(\mathbf{x}_t \in \ell^2(\mathcal{V})\right)_{t \in \mathbb{Z}}, \qquad (1)$$

elements in a Hilbert space $\mathcal{H} = \ell^2(\mathbb{Z} \times \mathcal{V})$.

Graph-shift operators of time-varying graph signals are bounded linear transformations on $\mathcal{H}$. Any $\mathbf{S} \in \mathcal{B}(\mathcal{H})$ has a unique kernel function, $\mathbf{K} : \mathbb{Z} \times \mathbb{Z} \to \mathcal{B}(\ell^2(\mathcal{V}))$ such that

$$(\mathbf{S}\mathbf{x})_t = \lim_{N \to \infty} \sum_{s=-N}^{N} \mathbf{K}(t,s)\mathbf{x}_s. \qquad (2)$$

We consider Laurent graph-shift operators $\mathbf{S} \in \mathcal{B}(\mathcal{H})$, *i.e.* $\mathbf{K}(t,s) = \mathbf{K}(t+d, s+d) = \mathbf{K}_{t-s}$ for all $d \in \mathbb{Z}$,

$$\mathbf{S}\mathbf{x} = \begin{bmatrix} \ddots & \ddots & \ddots & & \\ \cdots & \mathbf{K}_0 & \mathbf{K}_{-1} & \mathbf{K}_{-2} & \\ \cdots & \mathbf{K}_1 & \mathbf{K}_0 & \mathbf{K}_{-1} & \cdots \\ & \mathbf{K}_2 & \mathbf{K}_1 & \mathbf{K}_0 & \cdots \\ & & \ddots & \ddots & \ddots \end{bmatrix} \begin{bmatrix} \vdots \\ \mathbf{x}[-1] \\ \mathbf{x}[0] \\ \mathbf{x}[1] \\ \vdots \end{bmatrix}, \qquad (3)$$

for which we recover a variant of the convolution theorem:

$$\sum_{t \in \mathbb{Z}} e^{2\pi i \omega t} (\mathbf{S}\mathbf{x})_t = \left(\sum_{s \in \mathbb{Z}} e^{2\pi i \omega s} \mathbf{K}_s\right) \cdot \left(\sum_{t \in \mathbb{Z}} e^{2\pi i \omega t} \mathbf{x}_t\right). \qquad (4)$$

The kernels capture the weighted edges between nodes at fixed timescales, *i.e.* $[\mathbf{K}_t]_{i,j}$ is the weighted edge from node j to node i at timescale t.

Pointwise for $\omega \in [0,1]$, we have a Jordan spectral representation

$$\sum_{s \in \mathbb{Z}} e^{2\pi i \omega s} \mathbf{K}_s = \sum_{k=0}^{m(\omega)} \lambda_k(\omega) \mathbf{P}_k(\omega) + \mathbf{N}_k(\omega) \qquad (5)$$

where $0 < m(\omega) \leq n$. The spectrum of $\mathbf{S}$ is $\Lambda(\mathbf{S}) = \cup_{\omega \in [0,1]} \{\lambda_k(\omega)\}_{k=0}^{m}$.

Example

Goal

Let $\mathbf{S} \in \mathcal{B}(\mathcal{H})$ be as in Fig. 2, where $\mathbf{K}$ is given by the weighted edges of the graph. We want to design an ideal bandpass filter $\mathbf{A} \in \mathcal{B}(\mathcal{H})$ according to (8) which passes only a single invariant subspace of $\mathbf{S}$.

$\mathbf{S}$ has a Jordan spectral representation given pointwise for $\omega \in [0,1]$ as in (5):

$$\lambda_{\pm}(\omega) = \frac{2}{5}e^{2\pi i \omega} \pm \sqrt{\left(1 - \frac{3}{5}e^{6\pi i \omega}\right)\left(1 - \frac{4}{5}e^{4\pi i \omega}\right)};$$

$$\mathbf{P}_{\pm}(\omega) = \frac{1}{2}\begin{bmatrix} 1 & \pm\sqrt{\frac{5-4e^{4\pi i \omega}}{5-3e^{6\pi i \omega}}} \\ \pm\sqrt{\frac{5-3e^{6\pi i \omega}}{5-4e^{4\pi i \omega}}} & 1 \end{bmatrix}; \text{ and}$$

$$\mathbf{N}_{\pm}(\omega) = \mathbf{0}.$$

Each element of $\Lambda(\mathbf{S})$ corresponds to an invariant subspace of $\mathbf{S}$, defined by the projections, $\mathbf{P}_{\pm}(\omega)$. These invariant subspaces are like modes in $\mathcal{H}$. As shown in Fig. 1, $\Lambda(\mathbf{S})$ is disjoint. Thus, we can choose ϕ holomorphic such that $\phi|_{U_-}$ and $\phi|_{U_+}$ do not need an analytic continuation on $\mathbb{C} \setminus U$.

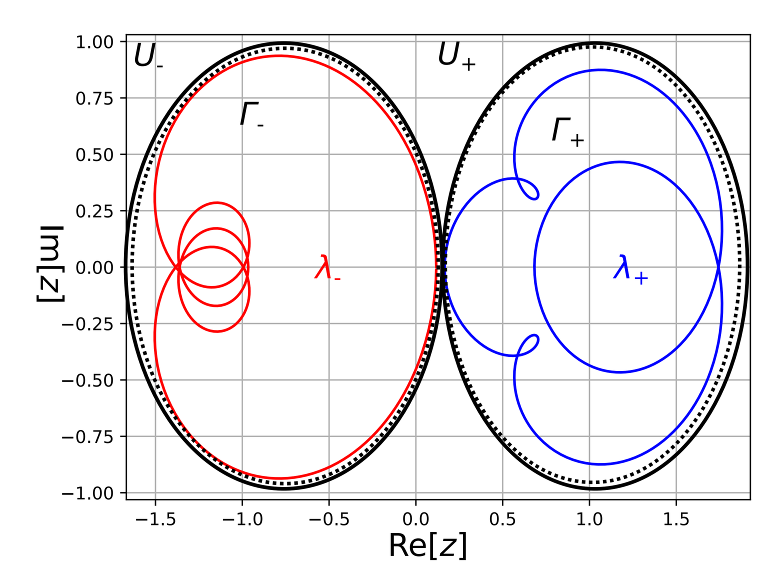

Figure 1: Spectrum of $\mathbf{S}$

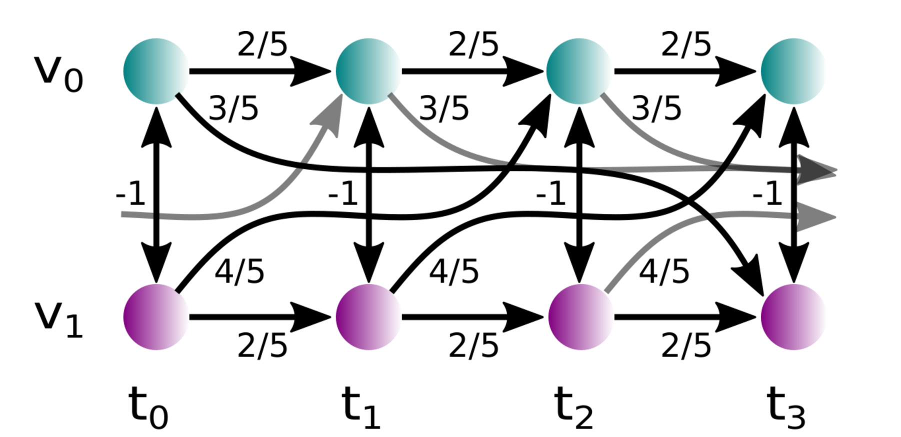

Figure 2: Graphical depiction of $\mathbf{S}$.

Let $\mathbf{A} = \lim_{\sigma \to 0} \phi(\mathbf{S}; \mu, \sigma)$ where ϕ is a circular complex Gaussian,

$$\phi(z; \mu, \sigma) = \begin{cases} \frac{1}{2\pi\sigma} \exp\left\{-\frac{1}{\sigma^2}|z-\mu|^2\right\} & z \in U_+ \\ 0 & o.w. \end{cases},$$

with $\mu \in \mathbb{C}$, $\sigma \in \mathbb{R}$, and U as defined in Fig. 1. Let $\mu = \lambda_+(\omega_0)$. Then, $\mathbf{A}$ implements an ideal bandpass,

$$(\mathbf{A}\mathbf{x})_t = e^{-2\pi i \omega_0 t}\mathbf{P}_+(\omega_0)\left(\sum_{s \in \mathbb{Z}} e^{2\pi i \omega_0 s}\mathbf{x}_s\right).$$

Filtering Time-Varying Graph Signals

Let $\mathbf{S} \in \mathcal{B}(\mathcal{H})$ be Laurent with a Jordan spectral representation given by Eq. (5). For all $\mathbf{x} \in \mathcal{H}$, we want to find covariant graph filters $\mathbf{A} \in \mathcal{B}(\mathcal{H})$,

$$(\mathbf{A}\mathbf{S}\mathbf{x})_t = (\mathbf{S}\mathbf{A}\mathbf{x})_t. \qquad (6)$$

Let $U \subset \mathbb{C}$ be an open set such that $\Lambda(\mathbf{S}) \subset U$ and $\phi : U \to \mathbb{C}$ be a holomorphic function. Then, for a closed curve $\Gamma \subset U$ that encloses $\Lambda(\mathbf{S})$,

$$\phi(\mathbf{S}) := \frac{1}{2\pi i}\oint_{\Gamma} \phi(z)(z\mathbf{I} - \mathbf{S})^{-1} dz \qquad (7)$$

defines a bounded operator on $\mathcal{H}$. Then, $\mathbf{A} = \phi(\mathbf{S})$ satisfies (6) and

$$\sum_{t \in \mathbb{Z}} e^{2\pi i \omega t}(\mathbf{A}\mathbf{x})_t = \sum_{k=0}^{m(w)} \left[(\phi \circ \lambda_k)(\omega)\mathbf{P}_k(\omega) + (\phi' \circ \lambda_k)(\omega)\mathbf{N}_k(\omega)\right] \cdot \hat{\mathbf{x}}(\omega). \qquad (8)$$

Conclusion

- Laurent graph-shift operators offer a more expressive graphical model than factor graphs
- Learning complexity can be controlled by parameterization of holomorphic function ϕ
- Applications include network neuroscience, social network modeling, and sensor array processing
- Future work will focus on application of approach in a learning problem

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