Inferring Time-Varying Signals over Uncertain Graphs

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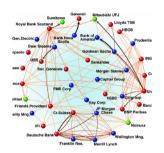
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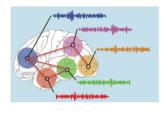
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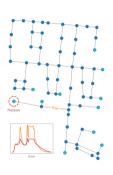


Multivariate Time Series over Networks





Brain recordings



Financial networks

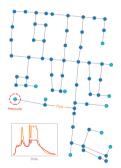
Water networks

Data have now a spatial dependency and a temporal dependency



Graphs for Multivariate Time Series

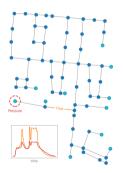
- ▶ Graphs can be used to model multivariate time series
 - \Rightarrow The structure is a graph
 - \Rightarrow Time series are time-varying data assigned to the nodes





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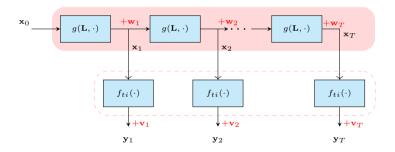


- \triangleright Nodes: junctions/sources in the city \mathcal{V}
- ightharpoonup Edges: pipes connecting the junctions $\mathcal E$
- Data: recorded pressure in each junction varying by time
 - $\Rightarrow \mathbf{x}_t$ over the graph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$ Shift op. (**A** or **L**)



State Space Model for Time-Varying Graph Signals $\frac{1}{2}$

$$\begin{cases} \mathbf{x}_t = g(\mathbf{L}, \mathbf{x}_{t-1}) + \mathbf{w}_{t-1} & \to \text{ state equation} \\ \mathbf{y}_t = f_t(\mathbf{L}, \mathbf{x}_t) + \mathbf{v}_t & \to \text{ observation equation} \end{cases}$$

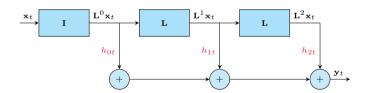




Observation Model: Graph Filter

- \triangleright We consider a graph filter at each time t for observation model
- ► Graph filter: shift-and-sum over the graph

$$\mathbf{y}_t = \sum_{k=0}^K \frac{\mathbf{h}_{kt}}{\mathbf{L}^k} \mathbf{x}_t = \mathbf{H}_t(\mathbf{L}) \mathbf{x}_t$$



▶ Goal: Learn h_{kt} to have a simple evolution in the state.



State Equation: Stochastic PDE over Graphs

- ▶ Strict PDE in the state: $\mathbf{H}_t(\mathbf{L})$ might not exist
 - ⇒ Hence, we allow some uncertainty in the state equation



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$$d\mathbf{x}_t = -c\mathbf{L}\mathbf{x}_t dt + \mathbf{S}d\boldsymbol{\beta}_t$$

- ${}^{\blacktriangleright}$ $\boldsymbol{\beta}_t \in \mathbb{R}^F$ is a standard Wiener process (a.k.a Brownian motion)
- ightharpoonup $\mathbf{S} \in \mathbb{R}^{N \times F}$ is the dispersion matrix



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- $ightharpoonup \mathbf{S} \in \mathbb{R}^{N \times F}$ is the dispersion matrix
- ightharpoonup Goal: Learn S \rightarrow has too many parameters
 - \Rightarrow We parameterize it by graph structure

$$\mathbf{S} = \mathbf{B} \mathrm{diag}(\boldsymbol{\alpha}) \longrightarrow d\mathbf{x}_t = -c \mathbf{L} \mathbf{x}_t dt + \mathbf{B} \mathrm{diag}(\boldsymbol{\alpha}) d\boldsymbol{\beta}_t$$

B is the incidence matrix



► Continuous-discrete state space model:

$$\begin{cases} d\mathbf{x}_t = -c\mathbf{L}\mathbf{x}_t dt + \mathbf{B} \operatorname{diag}(\boldsymbol{\alpha}) d\boldsymbol{\beta}_t \\ \mathbf{y}_t = \mathbf{H}_t(\mathbf{L})\mathbf{x}_t + \mathbf{v}_t \end{cases}$$



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- ightharpoonup initial state value: $\mathbf{x}_0 \sim \mathcal{N}(\boldsymbol{\mu}_0, \boldsymbol{\Sigma}_0)$
- ${\color{red} \blacktriangleright}$ noise energy: $\mathbb{E}[\mathbf{v}_k\mathbf{v}_k^{\top}]=\sigma^2\mathbf{I}$

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 - \Rightarrow given: temporal observations $\mathbf{y}_1, \dots, \mathbf{y}_T$
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- Approach:
- 1. Discretization of state
- 2. Recovering the state
- 3. Estimating model parameters



Step1: Discretization of Continuous State

▶ Using the transition matrix of an LTI-SPDE:

$$\mathbf{x}_{t+\triangle t} = \tilde{\mathbf{L}}\mathbf{x}_t + \mathbf{q}_t$$

with:

$$egin{aligned} \mathbf{q}_k &\sim \mathcal{N}(\mathbf{0}, \mathbf{Q}) \ & \tilde{\mathbf{L}} = \exp(-c \triangle t \mathbf{L}) \ & \mathbf{Q} = \int_0^{\triangle t} e^{-c \mathbf{L}(\triangle t - s)} \mathbf{B} \mathrm{diag}^2(\boldsymbol{\alpha}) \mathbf{B}^\top e^{-c \mathbf{L}(\triangle t - s)} ds \end{aligned}$$

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▶ With first-order Taylor approximation:

$$ilde{\mathbf{L}} pprox \mathbf{I} - c \triangle t \mathbf{L}$$

$$\mathbf{Q} pprox \triangle t \mathbf{B} \mathrm{diag}^2(\boldsymbol{\alpha}) \mathbf{B}^{\top}$$



Step2: Recovering the State

Kalman-Bucy filtering/smoothing

- \triangleright Given model parameters α and \mathbf{H}_t : state recovery via Kalman filtering
 - \Rightarrow optimum Bayesian solution (recursive closed form \rightarrow linear complexity in time)



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prediction step:

$$\begin{split} \mathbf{x}_t^{t-1} &= \tilde{\mathbf{L}} \mathbf{x}_{t-1}^{t-1}; \\ \mathbf{P}_t^{t-1} &= \tilde{\mathbf{L}} \mathbf{P}_{t-1}^{t-1} \tilde{\mathbf{L}} + \mathbf{B} \mathrm{diag}^2(\boldsymbol{\alpha}) \mathbf{B}^\top; \end{split}$$

- ightharpoonup K_t is the Kalman gain
- \triangleright $(\mathbf{y}_t \mathbf{H}_t \mathbf{x}_t^{t-1})$ is the prediction error
- $ightharpoonup \mathbf{P}_t$ is the covariance matrix of the state at time t

correction step:

$$\mathbf{K}_{t} = \mathbf{P}_{t}^{t-1} \mathbf{H}_{t}^{\top} (\mathbf{H}_{t} \mathbf{P}_{t}^{t-1} \mathbf{H}_{t}^{\top} + \sigma^{2} \mathbf{I})^{-1}$$

$$\mathbf{x}_{t}^{t} = \mathbf{x}_{t}^{t-1} + \mathbf{K}_{t} (\mathbf{y}_{t} - \mathbf{H}_{t} \mathbf{x}_{t}^{t-1});$$

$$\mathbf{P}_{t}^{t} = \mathbf{P}_{t}^{t-1} - \mathbf{K}_{t} \mathbf{P}_{t}^{t-1} \mathbf{K}_{t}^{\top};$$



Step3: Estimating Model Parameters

a maximum a priori approach

- \triangleright Having the state via Kalman filter \rightarrow likelihood on the observation
 - \Rightarrow can be even computed recursively!

$$\mathcal{L}_t(\boldsymbol{\alpha}, \mathbf{h}_t) = \mathcal{L}_{t-1}(\boldsymbol{\alpha}, \mathbf{h}_t) + \frac{1}{2} \log |\mathbf{S}_t|$$

$$+ \frac{1}{2} (\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t^{t-1})^{\top} \mathbf{S}_t^{-1} (\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t^{t-1})$$

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- rror matters more when confidence is high!
- ightharpoonup no l_2 -norm risk anymore ightharpoonup covariance-based norm replaced
- ▶ gradient descent and inference is over!

Experiments

▶ Datasets:

- ⇒ Synthetic data: based on presented state space model (200 nodes, 10000 samples)
- \Rightarrow Weather data: NOAA (109 nodes, \sim 8500 samples)
- \Rightarrow Traffic data: METR-LA (207 nodes, \sim 28000 samples)



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► Tasks:

- \Rightarrow Interpolation: randomly removing data over nodes at each time
- \Rightarrow Extrapolation: forecasting time series, using state equation



Interpolation

data imputation

Table: Interpolation task performance for both synthetic and weather temperature dataset. The experiments are performed based on different portions of unobserved data.

rNMSE	Synthetic			Weather			Traffic		
	10%	20%	30%	10%	20%	30%	10%	20%	30%
LMS	0.40	0.46	0.46	0.42	0.43	0.49	0.41	0.45	0.48
StarGP	0.31	0.31	0.36	0.25	0.24	0.31	0.21	0.25	0.29
G-SPDE	0.12	0.14	0.16	0.13	0.14	0.17	0.16	0.15	0.27
No - α	0.24	0.27	0.30	0.23	0.28	0.31	0.27	0.33	0.37
Fixed- α	0.24	0.26	0.29	0.22	0.26	0.29	0.24	0.27	0.36
Learn-S	0.23	0.20	0.20	0.21	0.21	0.27	0.19	0.22	0.34



Extrapolation forecasting

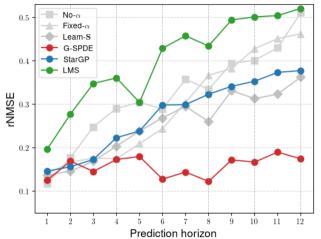


Figure. Traffic forecasting performance in rNMSE for proposed models with different prediction horizons.



Thanks for your attention!

