Inferring Time-Varying Signals over Uncertain Graphs

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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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- ▶ Nodes: junctions/sources in the city \mathcal{V}
- **Edges:** pipes connecting the junctions \mathcal{E}
- \blacktriangleright Data: recorded pressure in each junction varying by time

 $\Rightarrow \mathbf{x}_t$ over the graph $\mathcal{G} = \{\mathcal{V}, \mathcal{E}\}$







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





Observation Model: Graph Filter

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

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



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

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

 $\blacktriangleright~{\bf B}$ is the incidence matrix



▶ Continuous-discrete state space model:

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



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 - \Rightarrow given: temporal observations $\mathbf{y}_1, \ldots, \mathbf{y}_T$
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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:

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

with:

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



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▶ With first-order Taylor approximation:

$$\begin{split} \tilde{\mathbf{L}} &\approx \mathbf{I} - c \triangle t \mathbf{L} \\ \mathbf{Q} &\approx \triangle t \mathbf{B} \text{diag}^2(\boldsymbol{\alpha}) \mathbf{B}^\top \end{split}$$



Step2: Recovering the State Kalman-Bucy filtering/smoothing

- **b** 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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$$\begin{split} & \frac{\text{prediction step:}}{\mathbf{x}_t^{t-1} = \tilde{\mathbf{L}} \mathbf{x}_{t-1}^{t-1};} \\ & \mathbf{P}_t^{t-1} = \tilde{\mathbf{L}} \mathbf{P}_{t-1}^{t-1} \tilde{\mathbf{L}} + \mathbf{B} \text{diag}^2(\boldsymbol{\alpha}) \mathbf{B}^\top; \end{split}$$

 $\frac{\text{correction step:}}{\mathbf{K}_t = \mathbf{P}_t^{t-1} \mathbf{H}_t^{\top} (\mathbf{H}_t \mathbf{P}_t^{t-1} \mathbf{H}_t^{\top} + \sigma^2 \mathbf{I})^{-1} \\ \mathbf{x}_t^t = \mathbf{x}_t^{t-1} + \mathbf{K}_t (\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t^{t-1}); \\ \mathbf{P}_t^t = \mathbf{P}_t^{t-1} - \mathbf{K}_t \mathbf{P}_t^{t-1} \mathbf{K}_t^{\top};$

- \blacktriangleright **K**_t is the Kalman gain
- ($\mathbf{y}_t \mathbf{H}_t \mathbf{x}_t^{t-1}$) is the prediction error
- $\blacktriangleright~{\bf P}_t$ is the covariance matrix of the state at time t



Step3: Estimating Model Parameters

 \blacktriangleright Having the state via Kalman filter \rightarrow likelihood on the observation

 \Rightarrow can be even computed recursively!

$$\begin{aligned} \mathcal{L}_t(\boldsymbol{\alpha}, \mathbf{h}_t) &= \mathcal{L}_{t-1}(\boldsymbol{\alpha}, \mathbf{h}_t) + \frac{1}{2} \log |\mathbf{S}_t| \\ &+ \frac{1}{2} (\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t^{t-1})^\top \mathbf{S}_t^{-1} (\mathbf{y}_t - \mathbf{H}_t \mathbf{x}_t^{t-1}) \end{aligned}$$

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error matters more when confidence is high!

- \blacktriangleright no $l_2\text{-norm}$ risk anymore \rightarrow covariance-based norm replaced
- ▶ gradient descent and inference is over!



Experiments

- ► Datasets:
 - \Rightarrow Synthetic data: based on presented state space model (200 nodes, 10000 samples)
 - \Rightarrow Weather data: NOAA (109 nodes, ~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: for ecasting 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
$\text{Learn-}\mathbf{S}$	0.23	0.20	0.20	0.21	0.21	0.27	0.19	0.22	0.34







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



Thanks for your attention!

