Machine Learning and Optimization for Understanding Spatiotemporal Systems

Time Series Imputation & Periodicity Quantification

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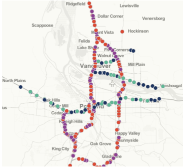
May 22, 2025

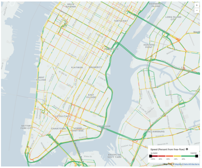
Orlando, USA

Spatiotemporal Data

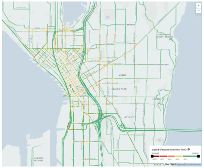
- Transport & mobility & climate application scenarios



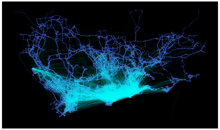
Highway (Portland)



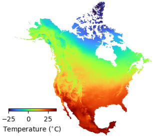
Uber movement (NYC)



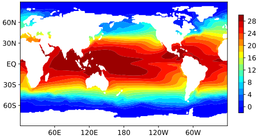
Uber movement (Seattle)



Taxi trajectory (Shenzhen)



Temperature (NA)



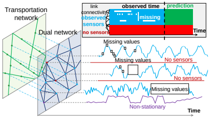
Temperature (sea surface)

- Challenges: Sparsity, high-dimensionality (network-scale), and multi-dimensionality (complicated data structure), time-varying systems

Research Contributions

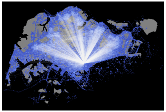
- (Practical) Formulating challenging spatiotemporal problems

Traffic Imputation — Mobility Pattern Discovery — Climate Seasonality Qualification



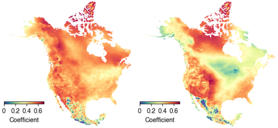
Missing data in transport

Matrix/tensor decomposition
Temporal dynamics



Singapore movement

Dynamical system modeling
Tensor decomposition

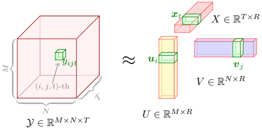


2000s 2010s

Interpretable ML
Mixed-integer programming

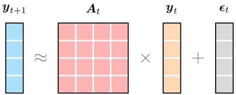
- (Methodological) Advancing ML development

Tensor decomposition



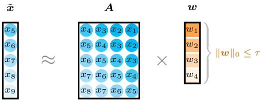
Integrate traffic flow patterns

Dynamic mode decomposition



Formulate dynamic patterns

Sparse autoregression



Interpret sparse autocorrelations

Reproducible Research

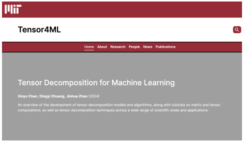
- The last mile of AI for spatiotemporal data computing

Human mobility & smart cities
Data-driven transport analytics
Spatiotemporal data modeling
Tensor decomposition for ML
Optimization for interpretable ML
. . .

Directions & Topics **Reproducible Research**

- Advancing ML development with open-source research

transdim
(1,200+ GitHub stars)
ML for Transport Data Imputation
https://github.com/xinychen/transdim

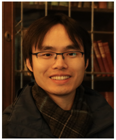


Tensor Decomposition for ML
(ML project)
Math & ML Tutorials
https://sites.mit.edu/tensor4ml

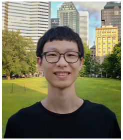
Spatiotemporal Data Computing
(Data valorization project)
Model Development of ML & Data Science
https://spatiotemporal-data.github.io

Spatiotemporal Data Imputation

❒ Convolution ❒ Fast Fourier transform ❒ Optimization w/ ℓ_1-norm
❒ Time series imputation ❒ Speed field reconstruction

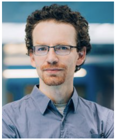


Xinyu Chen
UdeM → MIT



Zhanhong Cheng
McGill → UF

HanQin Cai
UCF



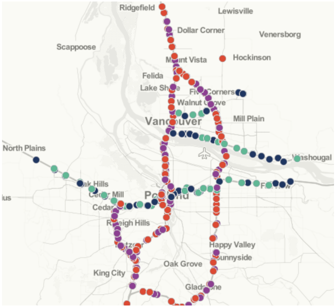
Nicolas Saunier
PolyMtl

Lijun Sun
McGill

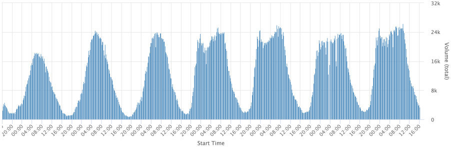
- **Xinyu Chen**, Zhanhong Chen, HanQin Cai, Nicolas Saunier, Lijun Sun (2024). "Laplacian Convolutional Representation for Traffic Time Series Imputation". *IEEE Transactions on Knowledge and Data Engineering*, 36 (11): 6490–6502.
- Blog post: Understanding time series convolution. https://spatiotemporal-data.github.io/posts/ts_conv

Motivation

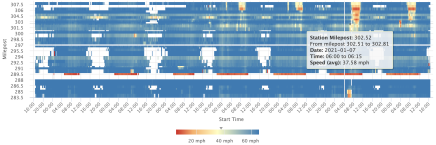
- Portland highway traffic data[1]



Highway network & sensor locations



Traffic volume

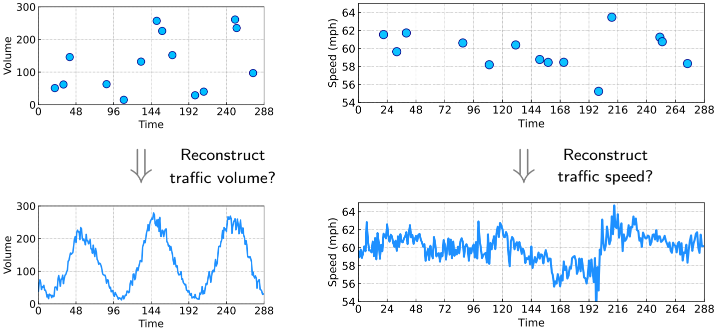


Traffic speed

- $\boldsymbol{X} \in \mathbb{R}^{N \times T}$ with N spatial locations $\times$ T time steps
- Traffic volume/speed shows strong spatial/temporal dependencies
- Missing data are there, how to improve data quality?

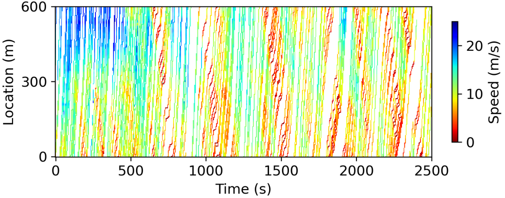
[1] https://portal.its.pdx.edu/home

Motivation

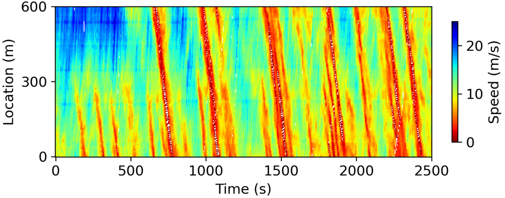


- How to utilize the global trends of traffic time series?
- How to produce local consistency of traffic data?

Motivation



200-by-500 matrix (NGSIM) $\Downarrow$ Reconstruct speed field from 20% sparse trajectories?

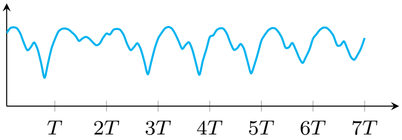


- How to learn from sparse spatiotemporal data?
- How to characterize spatial/temporal local dependencies?

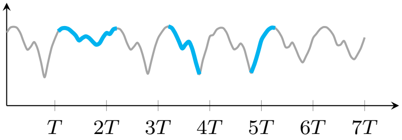
Time Series Imputation

Global/local trends in sparse data?

- Global trends (e.g., daily/weekly periodicity):

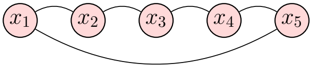


- Local trends (e.g., short-term time series trends):



Local Trend Modeling

- Intuition of Laplacian matrix



Undirected and circulant graph

$$\xrightarrow{\text{Modeling}} \quad \boldsymbol{L} = \begin{bmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{bmatrix}$$

(Circulant) Laplacian matrix

- Laplacian kernel:

$$\boldsymbol{\ell} \triangleq \underbrace{(2, -1, 0, 0, -1)^\top}_{\text{first column of } \boldsymbol{L}}$$

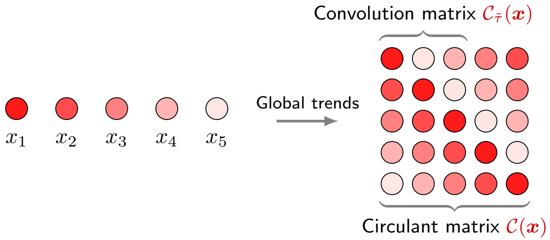
extending to the degree 2τ (i.e., graph connectivity) for $\boldsymbol{x} \in \mathbb{R}^T$.

- Temporal regularization:

$$\mathcal{R}(\boldsymbol{x}) = \underbrace{\frac{1}{2}\|\boldsymbol{L}\boldsymbol{x}\|_2^2}_{\text{mat-vec mul.}} = \underbrace{\frac{1}{2}\|\boldsymbol{\ell} \star \boldsymbol{x}\|_2^2}_{\text{convolution } \star}$$

Global Trend Modeling

Circulant matrix $\mathcal{C}(\boldsymbol{x})$ vs. convolution matrix $\mathcal{C}_{\tilde{\tau}}(\boldsymbol{x})$



- Circulant/Convolution nuclear norm minimization
  - A balance between global and local trends modeling?

CircNNM (Liu'22, Liu & Zhang'23)

$$\min_{\boldsymbol{x}} \;\|\mathcal{C}(\boldsymbol{x})\|_*$$
$$\text{s.t. } \|\mathcal{P}_\Omega(\boldsymbol{x}-\boldsymbol{y})\|_2 \leq \epsilon$$

on data $\boldsymbol{y}$ w/ observed index set Ω.

ConvNNM (Liu'22, Liu & Zhang'23)

$$\min_{\boldsymbol{x}} \;\|\mathcal{C}_{\tilde{\tau}}(\boldsymbol{x})\|_*$$
$$\text{s.t. } \|\mathcal{P}_\Omega(\boldsymbol{x}-\boldsymbol{y})\|_2 \leq \epsilon$$

on data $\boldsymbol{y}$ w/ observed index set Ω.

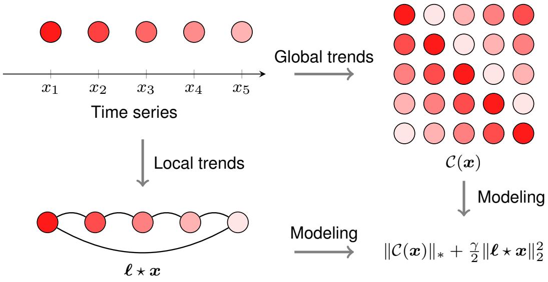
Global + Local Trends?

Laplacian Convolutional Representation (LCR)

For any partially observed time series $\boldsymbol{y} \in \mathbb{R}^T$ with observed index set Ω, LCR utilizes circulant matrix and Laplacian kernel to characterize global/local time series trends:

$$\min_{\boldsymbol{x}} \; \underbrace{\|\mathcal{C}(\boldsymbol{x})\|_*}_{\text{global}} + \frac{\gamma}{2} \underbrace{\|\boldsymbol{\ell} \star \boldsymbol{x}\|_2^2}_{\text{local}}$$

$$\text{s.t. } \|\mathcal{P}_\Omega(\boldsymbol{x} - \boldsymbol{y})\|_2 \leq \epsilon$$



Laplacian Convolutional Representation

- LCR model:

$$\begin{aligned}\min_{\boldsymbol{x}}\ & \|\mathcal{C}(\boldsymbol{x})\|_* + \frac{\gamma}{2}\|\boldsymbol{\ell}\star\boldsymbol{x}\|_2^2 \\ \text{s.t. } & \|\mathcal{P}_\Omega(\boldsymbol{x}-\boldsymbol{y})\|_2 \leq \epsilon\end{aligned}$$

$$\Longrightarrow \quad \begin{aligned}\min_{\boldsymbol{x}}\ & \underbrace{\|\mathcal{C}(\boldsymbol{x})\|_* + \frac{\gamma}{2}\|\boldsymbol{\ell}\star\boldsymbol{x}\|_2^2}_{\text{global + local}} + \underbrace{\frac{\eta}{2}\|\mathcal{P}_\Omega(\boldsymbol{z}-\boldsymbol{y})\|_2^2}_{\text{regularization}} \\ \text{s.t. } & \boldsymbol{z}=\boldsymbol{x}\end{aligned}$$

"The alternating direction method of multipliers (ADMM) is an algorithm that solves convex optimization problems by breaking them into smaller pieces, each of which are then easier to handle."

— Source: https://stanford.edu/~boyd/admm.html

Laplacian Convolutional Representation

- Augmented Lagrangian function:

$$\mathcal{L}=\underbrace{\|\mathcal{C}(\boldsymbol{x})\|_*+\frac{\gamma}{2}\|\boldsymbol{\ell}\star\boldsymbol{x}\|_2^2}_{\text{global + local}}+\underbrace{\frac{\lambda}{2}\|\boldsymbol{x}-\boldsymbol{z}\|_2^2+\langle\boldsymbol{w},\boldsymbol{x}-\boldsymbol{z}\rangle}_{\text{Lagrangian multiplier } \boldsymbol{w}}+\underbrace{\frac{\eta}{2}\|\mathcal{P}_{\Omega}(\boldsymbol{z}-\boldsymbol{y})\|_2^2}_{\text{observations } \boldsymbol{y}}$$

- Optimize $\boldsymbol{x}$ w/ FFT in $\mathcal{O}(T\log T)$ time: :

$$\begin{cases}\|\mathcal{C}(\boldsymbol{x})\|_*=\|\mathcal{F}(\boldsymbol{x})\|_1=\|\hat{\boldsymbol{x}}\|_1 & \text{(circulant matrix)}\\ \frac{1}{2}\|\boldsymbol{\ell}\star\boldsymbol{x}\|_2^2=\frac{1}{2T}\|\mathcal{F}(\boldsymbol{\ell})\circ\mathcal{F}(\boldsymbol{x})\|_2^2=\frac{1}{2T}\|\hat{\boldsymbol{\ell}}\circ\hat{\boldsymbol{x}}\|_2^2 & \text{(circular convolution)}\end{cases}$$

- Reformulate the optimization as ℓ_1-norm minimization:

$$\boldsymbol{x}:=\arg\min_{\boldsymbol{x}}\;\|\mathcal{C}(\boldsymbol{x})\|_*+\frac{\gamma}{2}\|\boldsymbol{\ell}\star\boldsymbol{x}\|_2^2+\frac{\lambda}{2}\|\boldsymbol{x}-\boldsymbol{z}+\boldsymbol{w}/\lambda\|_2^2$$

$$\Longrightarrow\hat{\boldsymbol{x}}:=\arg\min_{\hat{\boldsymbol{x}}}\;\underbrace{\|\hat{\boldsymbol{x}}\|_1}_{\ell_1\text{-norm}}+\frac{\gamma}{2T}\|\hat{\boldsymbol{\ell}}\circ\hat{\boldsymbol{x}}\|_2^2+\frac{\lambda}{2T}\|\hat{\boldsymbol{x}}-\hat{\boldsymbol{z}}+\hat{\boldsymbol{w}}/\lambda\|_2^2$$

Laplacian Convolutional Representation

ℓ_1-norm Minimization (Liu & Zhang'23)

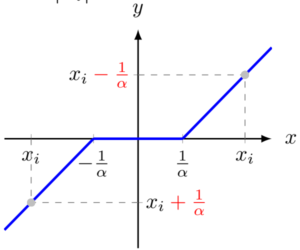
For any $\hat{\boldsymbol{h}} \in \mathbb{C}^T$ and $\delta \in \mathbb{R}$:

$$\min_{\hat{\boldsymbol{x}}} \;\|\hat{\boldsymbol{x}}\|_1 + \frac{\delta}{2}\|\hat{\boldsymbol{x}} - \hat{\boldsymbol{h}}\|_2^2$$

The solution to $\hat{\boldsymbol{x}}$:

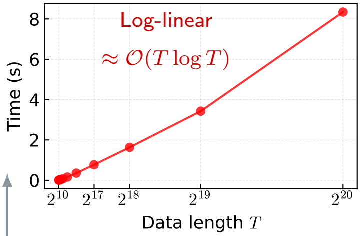
$$\hat{x}_t := \frac{\hat{h}_t}{|\hat{h}_t|} \cdot \underbrace{\max\{0, |\hat{h}_t| - 1/\delta\}}_{\text{shrinkage (e.g., ReLU)}}, t \in [T]$$

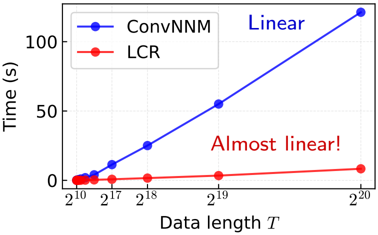
$$y_i = \frac{x_i}{|x_i|} \cdot \max\{|x_i| - 1/\alpha, 0\}$$



Laplacian Convolutional Representation

Time complexity & scalability & efficiency?



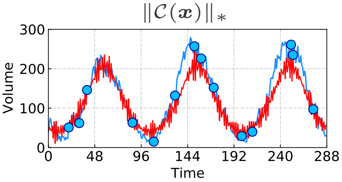


Empirical time complexity

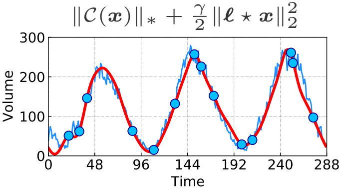
On the synthetic data $\boldsymbol{y} \in \mathbb{R}^T$ with $T \in \{2^{10}, 2^{11}, \ldots, 2^{20}\}$

Experiments

- Traffic speed imputation[2] (95% missing rate)



$\Downarrow$ Plus **local** time series trends



Highlights:

- Rethink the importance of local trend modeling in traffic data imputation tasks.
- Find a unified global and local trend modeling framework whose optimization can be efficiently solved by FFT:

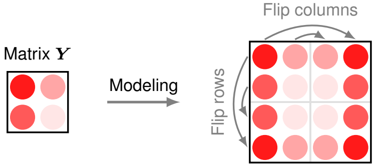
$$\min_{\boldsymbol{x}} \ \underbrace{\|\mathcal{C}(\boldsymbol{x})\|_*}_{\text{global}} + \frac{\gamma}{2} \underbrace{\|\boldsymbol{\ell} \star \boldsymbol{x}\|_2^2}_{\text{local}}$$
$$\text{s.t.} \ \ \|\mathcal{P}_\Omega(\boldsymbol{x} - \boldsymbol{y})\|_2 \leq \epsilon$$

[2] Blue dot: partial observation; red line: imputation.

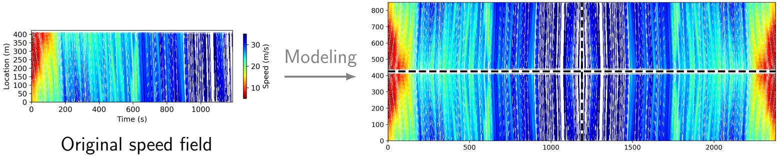
Experiments

Speed field reconstruction[3]

- Flipping operation on a matrix:



- Flipping operation on a speed field of vehicular traffic flow:



Original speed field

Flipped speed field

[3]Highway Drone (HighD) dataset at https://www.highd-dataset.com/

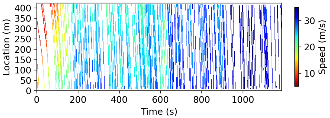
Experiments

Speed field reconstruction in German highways[4]

- Scenario: Mask trajectories of 70% vehicles
- LCR-2D on partially observed $\boldsymbol{Y} \in \mathbb{R}^{N \times T}$:

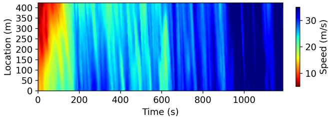
$$\min_{\boldsymbol{X}} \quad \underbrace{\|\mathcal{C}(\boldsymbol{X})\|_*}_{\text{global trend}} + \frac{\gamma}{2} \underbrace{\|(\boldsymbol{\ell}_s \boldsymbol{\ell}^\top) \star \boldsymbol{X}\|_F^2}_{\text{local trend}}$$

$$\text{s.t. } \|\mathcal{P}_\Omega(\boldsymbol{X} - \boldsymbol{Y})\|_F \leq \epsilon$$

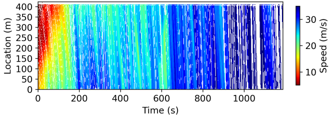


Sparse speed field

LCR-2D



Reconstructed speed field



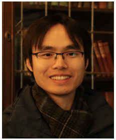
Ground-truth speed field

[4]Highway Drone (HighD) dataset at https://www.highd-dataset.com/

Quantifying Time Series Periodicity

(Ongoing Research)

❐ Interpretable ML ❐ Optimization w/ ℓ_0-norm ❐ Mixed-integer programming
❐ Human mobility regularity ❐ Climate system seasonality



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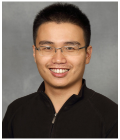
HanQin Cai
UCF

Ryan Qi Wang
Northeastern



Lijun Ding
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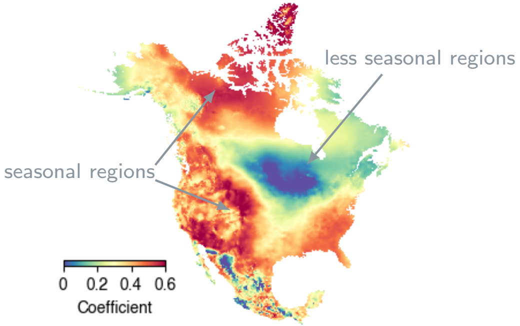
BU

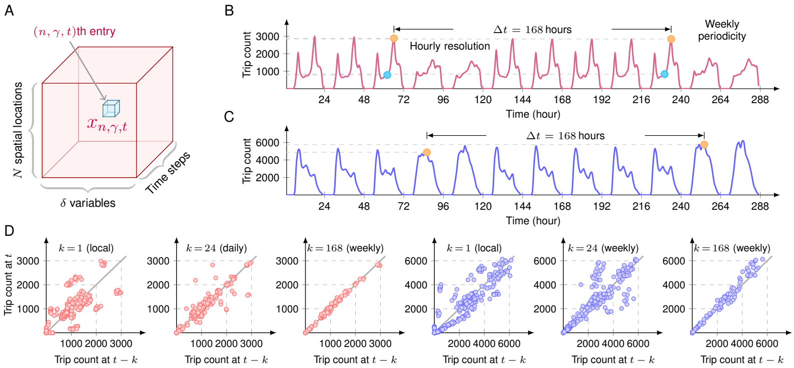
Motivation



Yearly temperature **seasonality** pattern in 2010s

Motivation

Human mobility data show daily/weekly regularity and periodicity?

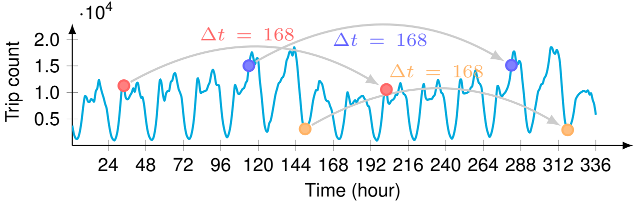


"**Closeness**" to the anti-diagonal $y = x$

$x_t \approx x_{t-168}$ (weekly periodicity)

Motivation

Weekly periodicity of ridesharing trip time series in Chicago



What motivate us most about **periodicity**?

❶ **Resilience and stability of systems**: Empirically measure the periodicity and predictability of urban systems.

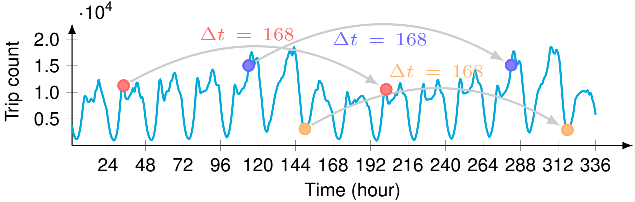
❷ **Optimization of transport systems**: Optimize resources (e.g., public transit, taxi, rideshare, and micromobility) to meet transport demand efficiently.

❸ **Design of sustainable transport & infrastructure**: Implement energy-efficient solutions tailored to peak hours.

Motivation

- Time series autoregression on $\boldsymbol{x} \in \mathbb{R}^T$

$$\boldsymbol{w} := \arg\min_{\{w_k\}_{k\in[d]}} \sum_{t\in[d+1,T]} \Big(x_t - \sum_{k\in[d]} w_k x_{t-k}\Big)^2$$



Periodicity of rideshare trip time series

- Sparse coefficient vector $\mapsto$ **Interpretability**?

$$\boldsymbol{w} = (\underbrace{0.33}_{k=1}, 0, \cdots, 0, \underbrace{0.20}_{k=167}, \underbrace{0.46}_{k=168})^\top \in \mathbb{R}^{168}$$

Valorizing Autoregression

- Time series autoregression

$$\begin{aligned} \boldsymbol{w} &:= \arg\min_{\{w_k\}_{k\in[d]}} \sum_{t\in[d+1,T]} \Big(x_t - \sum_{k\in[d]} w_k x_{t-k}\Big)^2 \\ &= \arg\min_{\boldsymbol{w}} \|\tilde{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{w}\|_2^2 \end{aligned}$$

$$\overset{\tilde{\boldsymbol{x}}}{\begin{bmatrix} x_5 \\ x_6 \\ x_7 \\ x_8 \\ x_9 \end{bmatrix}} \approx \overset{\boldsymbol{A}}{\begin{bmatrix} x_4 & x_3 & x_2 & x_1 \\ x_5 & x_4 & x_3 & x_2 \\ x_6 & x_5 & x_4 & x_3 \\ x_7 & x_6 & x_5 & x_4 \\ x_8 & x_7 & x_6 & x_5 \end{bmatrix}} \times \overset{\boldsymbol{w}}{\begin{bmatrix} w_1 \\ w_2 \\ w_3 \\ w_4 \end{bmatrix}} \Big\} \|\boldsymbol{w}\|_0 \leq \tau$$

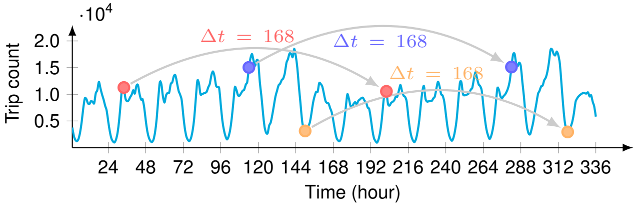
Autoregression on time series $\boldsymbol{x} = (x_1, x_2, \ldots, x_9)^\top$ w/ sparsity $\tau \in \mathbb{Z}^+$

- Sparse autoregression

$$\begin{aligned} &\min_{\boldsymbol{w}\geq 0} \ \|\tilde{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{w}\|_2^2 \\ &\text{s.t.} \ \underbrace{\|\boldsymbol{w}\|_0 \leq \tau}_{\text{sparsity w/ } \ell_0\text{-norm}} \end{aligned} \iff \begin{aligned} &\min_{\boldsymbol{w},\boldsymbol{\beta}} \ \|\tilde{\boldsymbol{x}} - \boldsymbol{A}\boldsymbol{w}\|_2^2 \\ &\text{s.t.} \ \begin{cases} 0 \leq \boldsymbol{w} \leq \boldsymbol{\beta}, \ \boldsymbol{\beta} \in \{0,1\}^d \\ \|\boldsymbol{\beta}\|_1 \leq \tau \end{cases} \end{aligned}$$

Solution Quality

- Subspace pursuit (SP) sometimes fails



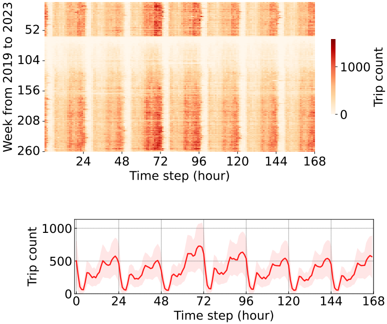
Periodicity of ridesharing trip time series

- Exact solution w/ mixed-integer programming (MIP)
- An intuitive example (sparsity $\tau = 2$):

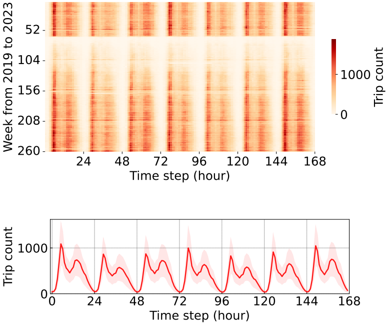
$$\underbrace{\boldsymbol{w} = (\cdots, \underbrace{0.02}_{k=53}, \cdots, \underbrace{0.96}_{k=168})^\top}_{\text{loss func.} = 8.32 \times 10^7 \text{ (SP)}} \quad \text{vs.} \quad \underbrace{\boldsymbol{w} = (\underbrace{0.22}_{k=1}, \cdots, \underbrace{0.77}_{k=168})^\top}_{\text{loss func.} = 6.25 \times 10^7 \text{ (MIP)}}$$

John F. Kennedy International Airport

- Pickup/Dropoff trips in airport
  - Pickup trips are relevant to flight delay, baggage claim, and other factors.
  - Dropoff trips to airport are highly related to flight schedules.



Pickup trips from airport



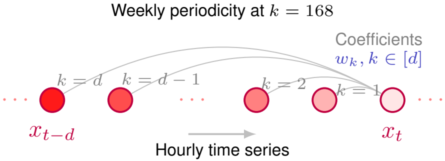
Dropoff trips to airport

- Sparse coefficient vectors (sparsity $\tau = 3$):

$$\boldsymbol{w} = (\underbrace{0.31}_{k=1}, \cdots, \underbrace{0.28}_{k=24}, \cdots, \underbrace{0.41}_{k=168})^\top \quad \text{vs.} \quad \boldsymbol{w} = (\underbrace{0.18}_{k=1}, \cdots, \underbrace{0.35}_{k=24}, \cdots, \underbrace{0.47}_{k=168})^\top$$

Spatially- and Time-Varying Autoregression

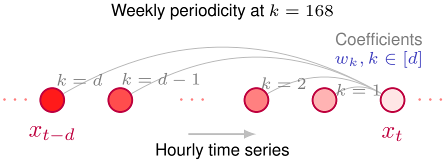
Univariate autoregression



$$\min \sum_{t} \Big(x_t - \sum_{k \in [d]} w_k x_{t-k} \Big)^2$$

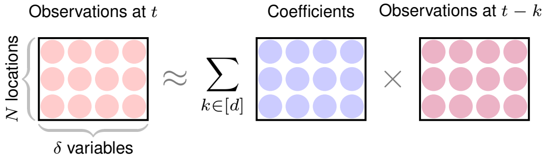
Spatially- and Time-Varying Autoregression

Univariate autoregression



$$\min \sum_{t} \Big(x_t - \sum_{k \in [d]} w_k x_{t-k} \Big)^2$$

Multidimensional autoregression



$$\min \sum_{n \in [N]} \sum_{\gamma \in [\delta]} \sum_{t} \Big(x_{n,\gamma,t} - \sum_{k \in [d]} w_{n,\gamma,k} x_{n,\gamma,t-k} \Big)^2$$

Envisioning Human Mobility

- Ridesharing trip data $\{\boldsymbol{x}_{n,\gamma}\}$ across $\gamma \in [\delta]$ years
- Reformulate sparse autoregression:

year

spatial location

hourly time step

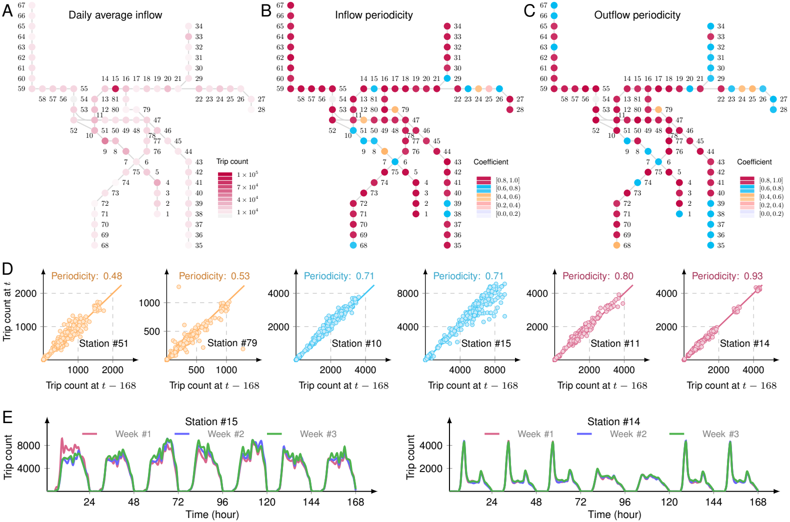
$$\min_{\{\boldsymbol{w}_{n,\gamma}\},\boldsymbol{\beta}} \sum_{n\in[N]} \sum_{\gamma\in[\delta]} \sum_{t\in[d+1,T_\gamma]} \Bigl(x_{n,\gamma,t} - \sum_{k\in[d]} w_{n,\gamma,k} x_{n,\gamma,t-k}\Bigr)^2$$

$$\text{s.t.} \quad \underbrace{\boldsymbol{\beta} \in \{0,1\}^d}_{\text{binary var.}} \quad \underbrace{0 \leq \boldsymbol{w}_{n,\gamma} \leq \boldsymbol{\beta}}_{\text{upper bound in } \{0,1\}} \quad \underbrace{\|\boldsymbol{\beta}\|_1 \leq \tau}_{\text{sum of binary var.}}$$

- MIP problem w/ $(N\delta + 1)d$ variables!
- How to handle thousands or millions of (e.g., $N\delta = 10^6$) time series?

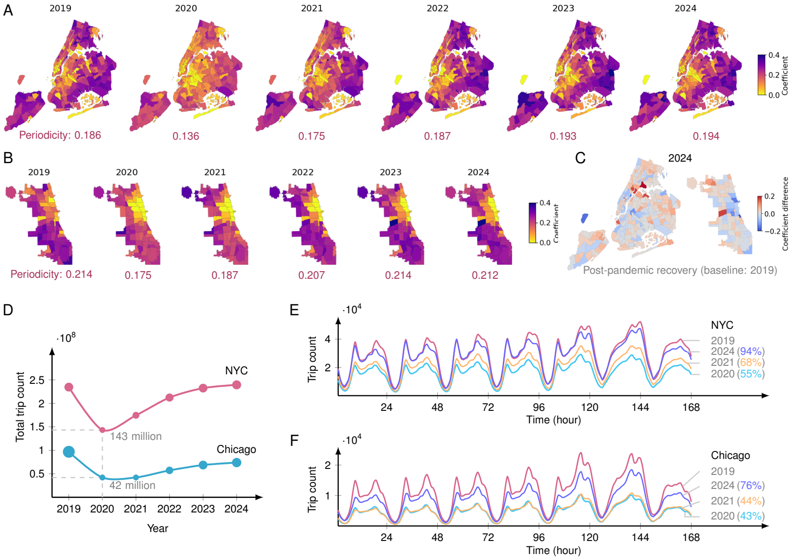
Quantify weekly periodicity by $\{w_{n,\gamma,k}\}$ at index $k = 168$

Envisioning Human Mobility



Hangzhou metro passenger flow in January 2019

Envisioning Human Mobility



Weekly periodicity reveals spatial patterns of ridesharing systems

Understanding Climate Systems

Quantify yearly seasonality by $\{w_{m,n,\gamma,k}\}$ at index $k = 12$

longitude

latitude　decade　monthly time step　temperature

$$\min_{\{\boldsymbol{w}_{m,n,\gamma}\},\boldsymbol{\beta}} \sum_{m\in[M]} \sum_{n\in[N]} \sum_{\gamma\in[\delta]} \sum_{t\in[d+1,T_\gamma]} \Big(x_{m,n,\gamma,t} - \sum_{k\in[d]} w_{m,n,\gamma,k} x_{m,n,\gamma,t-k} \Big)^2$$

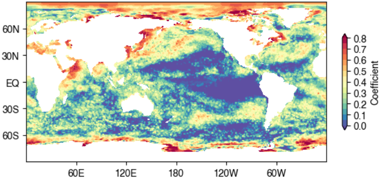
$$\text{s.t.} \begin{cases} \boldsymbol{\beta} \in \{0,1\}^d \\ 0 \leq \boldsymbol{w}_{m,n,\gamma} \leq \boldsymbol{\beta},\ \forall m,n,\gamma \\ \|\boldsymbol{\beta}\|_1 \leq \tau \\ \|\boldsymbol{w}_{m,n,\gamma}\|_1 = 1,\ \forall m,n,\gamma \end{cases}$$

binary decision var.

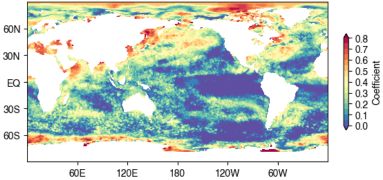
sparsity constraints

ℓ_1-normalization

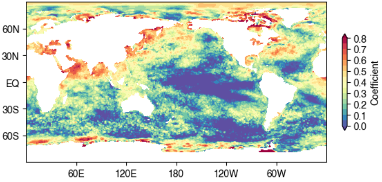
Sea Surface Temperature



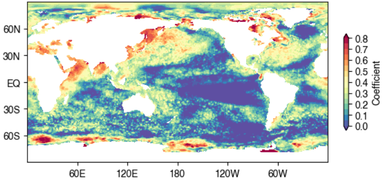
1980s



1990s



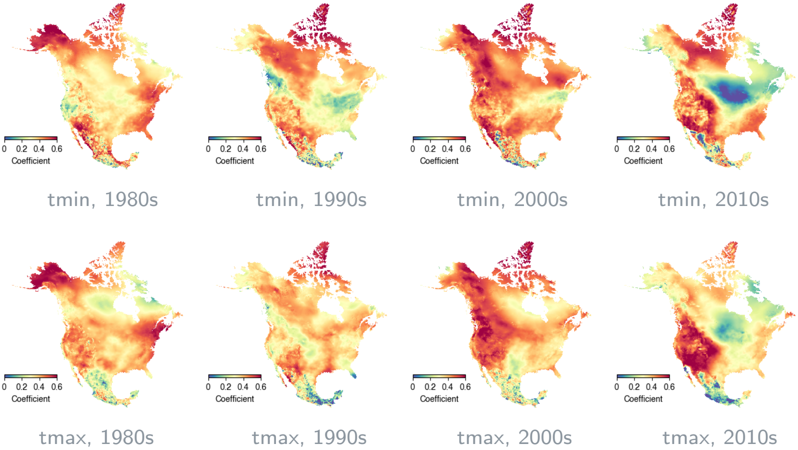
2000s



2010s

- Identify yearly periodicity at $k = 12$ from SST data ($\tau = 3$)
  1. The areas of El Nino events are less seasonal/predictable
  2. Arctic becomes less seasonal/predictable in the past 20 years
- Insights into climate system monitoring

North America Temperature



- Identify yearly periodicity at $k = 12$ from temperature data ($\tau = 3$)
  1. Stronger yearly seasonality in high-latitude areas
  2. Less seasonal temperature in south areas (e.g., Mexico)
  3. Seasonality patterns in 2000s & 2010s are different from 1980s & 1990s

Thanks for your attention!

Any Questions?

Slides: https://xinychen.github.io/slides/ml_opt_stsystem.pdf

Essential AR: https://xinychen.github.io/slides/essential_ar.pdf

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