



Machine Learning and Optimization for Data-Driven Transportation Analytics

Tensor Decomposition, Interpretable ML, Mathematical Programming

📍 School of Management, Technical University of Munich

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December 6, 2024

Transport Data

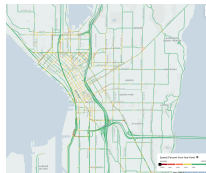
- Transport & mobility application scenarios



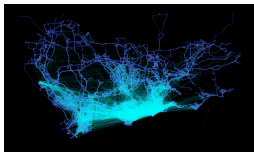
Highway (Portland)



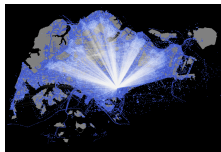
Uber movement (NYC)



Uber movement (Seattle)



Taxi trajectory (Shenzhen)



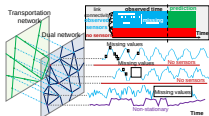
Human movement (Singapore)

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

Data-Driven Transportation Analytics

Part I

Traffic Imputation

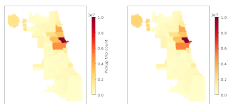


Chen et al.'24

Matrix/tensor completion
Circulant matrix
Circular convolution
Fast Fourier transform

Part II

Pattern Discovery

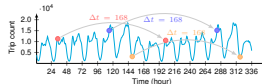


Chen et al.'24

Time series autoregression
Tensor decomposition
Conjugate gradient
Procrustes problems

Part III

Periodicity Qualification



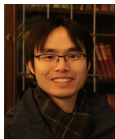
Working paper

Time series autoregression
Sparse learning
Greedy methods
Mixed-integer programming

ML + Optimization for Transportation

Spatiotemporal Traffic Data Imputation

(Matrix/Tensor Factorization)



Xinyu Chen
UdeM → MIT



Nicolas Saunier
PolyMtl

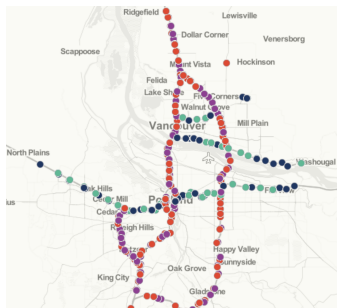


Lijun Sun
McGill

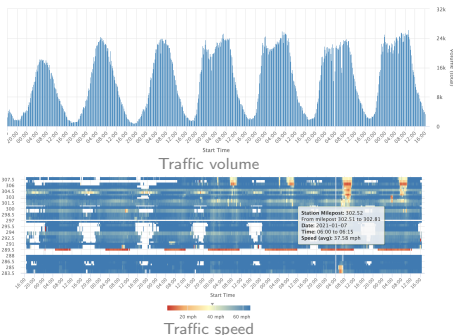
- **Chen & Sun (2022)**. “Bayesian Temporal Factorization for Multidimensional Time Series Prediction”. IEEE Transactions on Pattern Analysis and Machine Intelligence, 44 (9): 4659–4673.
- **Chen et al. (2024)**. “Laplacian Convolutional Representation for Traffic Time Series Imputation”. IEEE Transactions on Knowledge and Data Engineering, 36 (11): 6490–6502.
- **Chen et al. (2024)**. “Forecasting Urban Traffic States with Sparse Data Using Hankel Temporal Matrix Factorization”. INFORMS Journal on Computing.

Traffic Flow Data

- Portland highway traffic data¹



Highway network & sensor locations



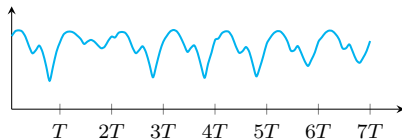
- $\mathbf{X} \in \mathbb{R}^{N \times T}$ with N spatial locations $\times T$ time steps
- Traffic volume/speed shows strong spatial/temporal dependencies
- Missing data are there, how to improve data quality?

¹<https://portal.its.pdx.edu/home>

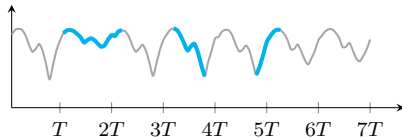
Time Series Imputation

Global/local trends in sparse data?

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

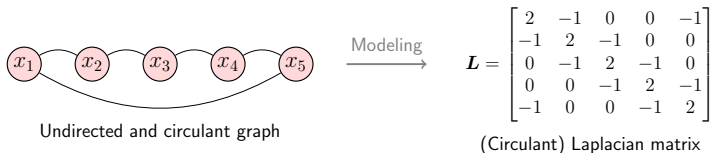


- Local trends (e.g., short-term time series trends):



Local Trend Modeling

- Intuition of Laplacian matrix



- Laplacian kernel:

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

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

- Temporal regularization:

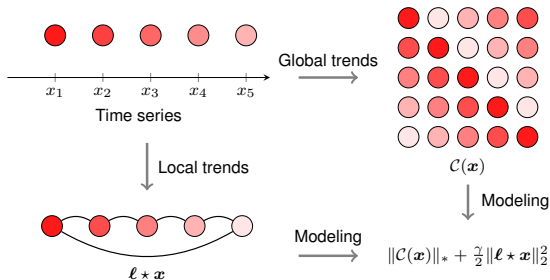
$$\mathcal{R}(x) = \underbrace{\frac{1}{2} \|Lx\|_2^2}_{\text{mat-vec mul.}} = \underbrace{\frac{1}{2} \|\ell \star x\|_2^2}_{\text{convolution } \star}$$

Global + Local Trends?

Laplacian Convolutional Representation (LCR)

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

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



Laplacian Convolutional Representation

- Augmented Lagrangian function:²

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

- Optimize $\mathbf{x}$ w/ FFT (Properties of circulant matrix & circular convolution)

$$\begin{cases} \|C(\mathbf{x})\|_* = \|\mathcal{F}(\mathbf{x})\|_1 = \|\hat{\mathbf{x}}\|_1 \\ \frac{1}{2}\|\ell \star \mathbf{x}\|_2^2 = \frac{1}{2T}\|\mathcal{F}(\ell) \circ \mathcal{F}(\mathbf{x})\|_2^2 = \frac{1}{2T}\|\hat{\ell} \circ \hat{\mathbf{x}}\|_2^2 \end{cases}$$

- Reformulate the optimization as ℓ_1 -norm minimization:

$$\begin{aligned} \mathbf{x} &:= \arg \min_{\mathbf{x}} \|C(\mathbf{x})\|_* + \frac{\gamma}{2}\|\ell \star \mathbf{x}\|_2^2 + \frac{\lambda}{2}\|\mathbf{x} - \mathbf{z} + \mathbf{w}/\lambda\|_2^2 \\ \Rightarrow \hat{\mathbf{x}} &:= \arg \min_{\hat{\mathbf{x}}} \underbrace{\|\hat{\mathbf{x}}\|_1}_{\ell_1\text{-norm}} + \frac{\gamma}{2T}\|\hat{\ell} \circ \hat{\mathbf{x}}\|_2^2 + \frac{\lambda}{2T}\|\hat{\mathbf{x}} - \hat{\mathbf{z}} + \hat{\mathbf{w}}/\lambda\|_2^2 \end{aligned}$$

in $\mathcal{O}(T \log T)$ time.

² $\mathbf{w} \in \mathbb{R}^T$ (Lagrange multiplier); $\langle \cdot, \cdot \rangle$ (inner product).

Laplacian Convolutional Representation

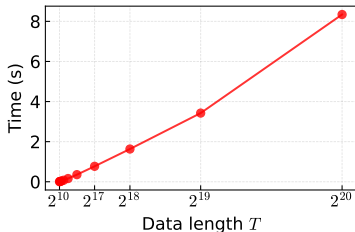
ℓ_1 -norm Minimization (Liu & Zhang'23)

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

with complex-valued $\hat{\mathbf{x}}, \hat{\mathbf{h}} \in \mathbb{C}^T$ and weight parameter δ , the solution is

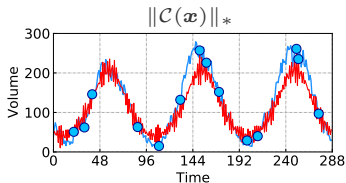
$$\hat{x}_t := \frac{\hat{h}_t}{|\hat{h}_t|} \cdot \underbrace{\max\{0, |\hat{h}_t| - 1/\delta\}}_{\text{shrinkage (e.g., ReLU)}}, t \in [T].$$

- **Empirical time complexity of LCR:** On the synthetic data $\mathbf{y} \in \mathbb{R}^T$ with $T \in \{2^{10}, 2^{11}, \dots, 2^{20}\}$ (w.r.t. FFT in $\mathcal{O}(T \log T)$ time)

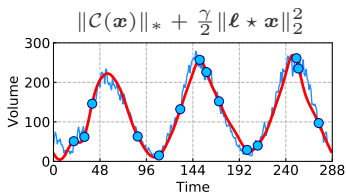


Experiments

- Traffic speed imputation³ (95% missing rate)



↓ 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**:

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

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

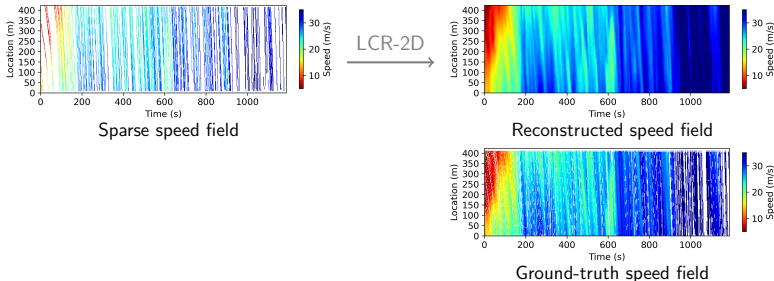
³Blue dot: partial observation; red line: imputation.

Experiments

Speed field reconstruction in German highways⁴

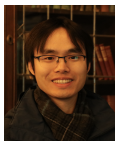
- Scenario: Mask trajectories of 70% vehicles
- LCR-2D on partially observed $\mathbf{Y} \in \mathbb{R}^{N \times T}$:

$$\min_{\mathbf{X}} \underbrace{\|\mathcal{C}(\mathbf{X})\|_*}_{\text{global trend}} + \frac{\gamma}{2} \underbrace{\|(\ell_s \ell^\top) \star \mathbf{X}\|_F^2}_{\text{local trend}}$$
$$\text{s.t. } \|\mathcal{P}_\Omega(\mathbf{X} - \mathbf{Y})\|_F \leq \epsilon$$



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

Discovering Dynamic Patterns from Spatiotemporal Systems



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HanQin Cai
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Shenhao Wang
UF

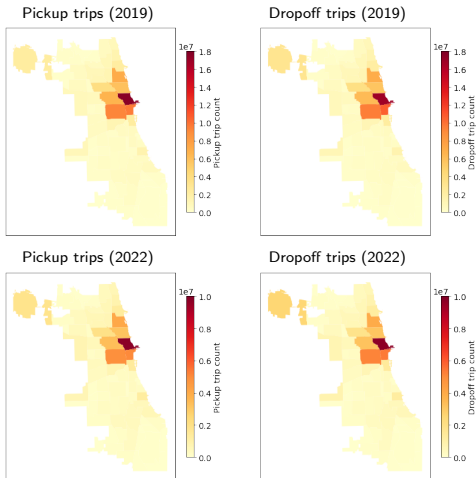


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- **Chen et al. (2024).** “Discovering Dynamic Patterns from Spatiotemporal Data with Time-Varying Low-Rank Autoregression”. *IEEE Transactions on Knowledge and Data Engineering*, 36 (2): 504–517.
- **Chen et al. (2025).** “Dynamic autoregressive tensor factorization for pattern discovery of spatiotemporal systems”. *IEEE Transactions on Pattern Analysis and Machine Intelligence*.

Motivation

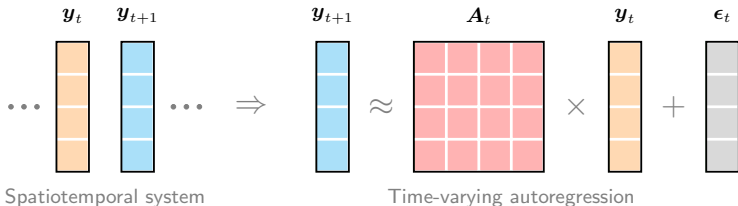
- Chicago rideshare: 96.6M trips (2019) vs. 57.3M trips (2022)



- Contradict:** No difference in aggregation. How about latent patterns?

Autoregression

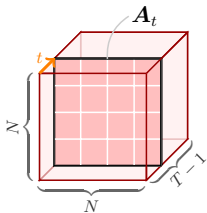
- How to characterize dynamical systems?

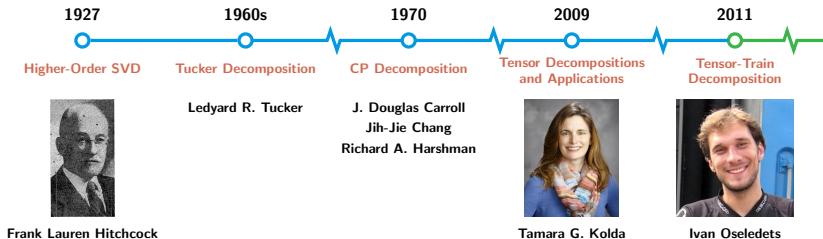


- On spatiotemporal data $\mathbf{Y} \in \mathbb{R}^{N \times T}$:

$$\underbrace{y_{t+1} = \mathbf{A} y_t + \epsilon_t}_{\text{time-invariant (e.g., DMD)}} \quad \text{v.s.} \quad \underbrace{y_{t+1} = \mathbf{A}_t y_t + \epsilon_t}_{\text{time-varying (ours)}}$$

- How to discover spatial/temporal modes (patterns) from the tensor $\mathcal{A} \triangleq \{\mathbf{A}_t\}_{t \in [T-1]}$?

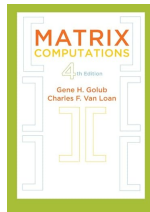




Dynamic Autoregressive Tensor Factorization

- Tensor factorization:

$$\begin{aligned} \mathcal{A} &= \underbrace{\mathcal{G} \times_1 \mathbf{W} \times_2 \mathbf{V} \times_3 \mathbf{X}}_{\text{Tucker decomposition}} \\ &\quad \Updownarrow \\ \mathbf{A}_t &= \mathcal{G} \times_1 \underbrace{\mathbf{W}}_{\text{spatial modes}} \times_2 \mathbf{V} \times_3 \underbrace{\mathbf{x}_t^\top}_{\text{temporal modes}} \end{aligned}$$



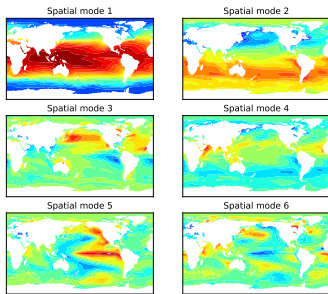
- Optimization problem:

$$\begin{aligned} \min_{\mathcal{G}, \mathbf{W}, \mathbf{V}, \mathbf{X}} \quad & \frac{1}{2} \sum_{t \in [T-1]} \|\mathbf{y}_{t+1} - (\mathcal{G} \times_1 \mathbf{W} \times_2 \mathbf{V} \times_3 \mathbf{x}_t^\top) \mathbf{y}_t\|_2^2 \\ \text{s.t.} \quad & \underbrace{\mathbf{W}^\top \mathbf{W}}_{\text{orthogonal spatial modes}} = \mathbf{I}_R \end{aligned}$$

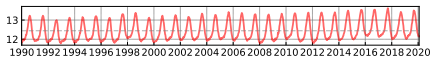
on spatiotemporal data $\mathbf{Y} \in \mathbb{R}^{N \times T}$.

Beyond Transport: Sea Surface Temperature

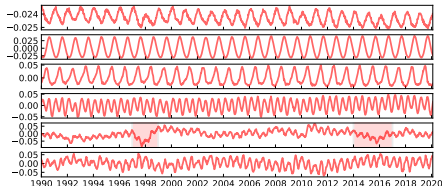
- Sea surface temperature (SST) dataset



Spatial modes in W



Time series of mean temperature

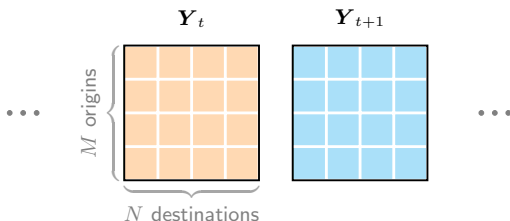


Temporal modes in X

- Identify two strongest El Nino events (on 1997-98 & 2014-16)
- Insights into climate change

Dynamic Autoregressive Tensor Factorization

- Origin-Destination (OD) matrices



- On spatiotemporal systems $\mathcal{Y} \in \mathbb{R}^{M \times N \times T}$:

$$\underbrace{\mathbf{y}_{n,t+1} = \mathbf{A}_{n,t} \mathbf{y}_{n,t} + \epsilon_{n,t}}_{\text{time-varying \& destination-varying}}$$

- Optimization problem:

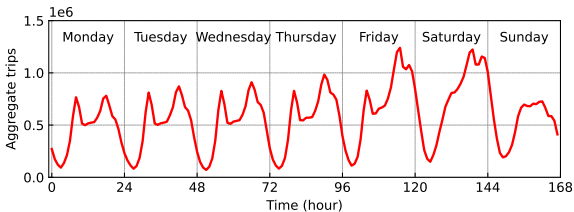
$$\min_{\mathcal{G}, \mathbf{W}, \mathbf{U}, \mathbf{V}, \mathbf{X}} \frac{1}{2} \sum_{n \in [N]} \sum_{t \in [T-1]} \left\| \mathbf{y}_{n,t+1} - \underbrace{(\mathcal{G} \times_1 \mathbf{W} \times_2 \mathbf{U} \times_3 \mathbf{V} \times_4 \mathbf{x}_t^\top)}_{\text{Tucker decomposition}} \mathbf{y}_{n,t} \right\|_2^2$$

s.t. $\underbrace{\mathbf{W}^\top \mathbf{W} = \mathbf{I}_R}_{\text{orthogonal origin patterns}}$

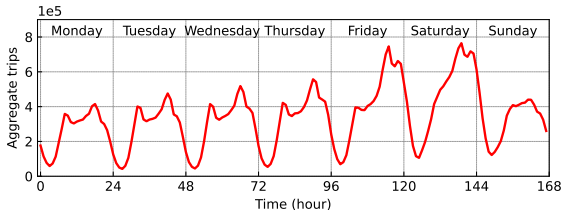
Human Mobility

- Chicago rideshare: 96.6M trips (2019) vs. 57.3M trips (2022)

Pickup trips aggregated over 52 weeks in 2019

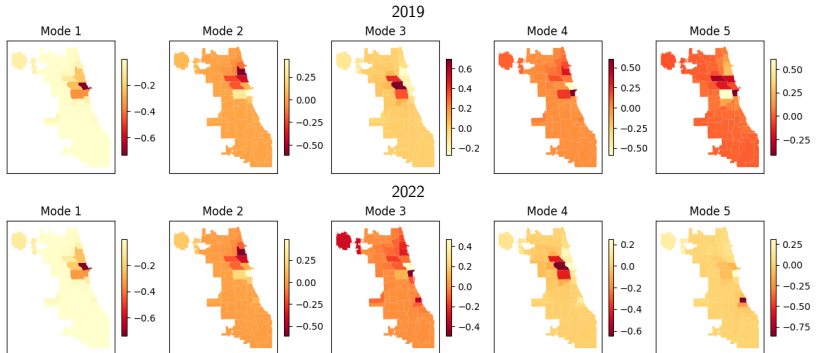


Pickup trips aggregated over 52 weeks in 2022



Human Mobility

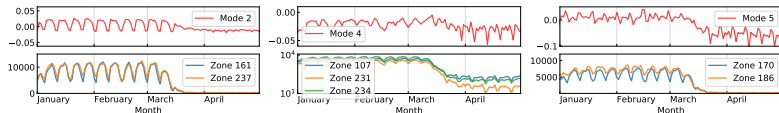
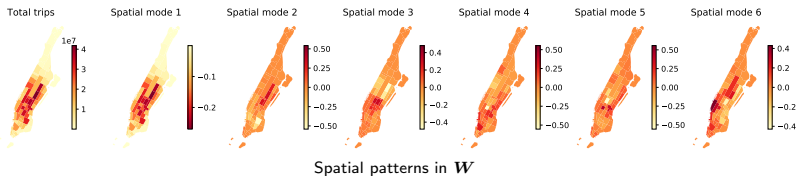
- Rideshare trip data: 77 origins $\times$ 77 destinations $\times$ 168 hours



- Identify the changes in pickup zones before/after COVID-19

Human Mobility

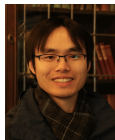
- NYC taxi dataset (pickup)
 - Remarkable decrease of trips due to COVID-19



- Identify the changes of temporal patterns due to COVID-19

Quantifying Periodicity of Human Mobility

(Working Ideas on Interpretable ML & Causality & Nonlinear Programming)



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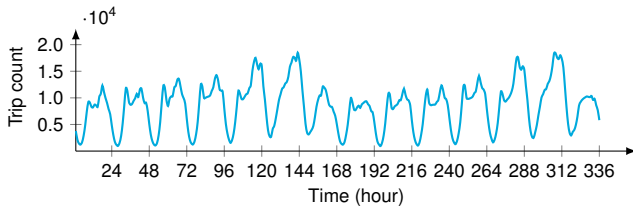


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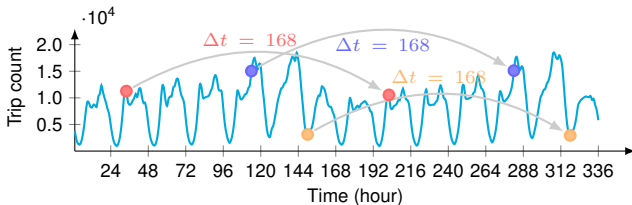
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Motivation



Two-week rideshare trip time series in Chicago since April 1, 2024

Motivation



Weekly periodicity of rideshare trip time series

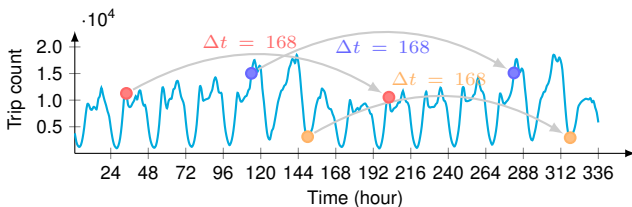
What motivate us most about **periodicity**?

- 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 $\mathbf{x} \in \mathbb{R}^T$

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



Periodicity of rideshare trip time series

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

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

Valorizing Autoregression

- Time series autoregression

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

The diagram illustrates the matrix equation $\tilde{\mathbf{x}} \approx \mathbf{A}\mathbf{w}$. The vector $\tilde{\mathbf{x}}$ contains elements x_5, x_6, x_7, x_8, x_9 . The matrix $\mathbf{A}$ is a 5x5 tridiagonal matrix with elements x_4, x_3, x_2, x_1 on the top row, x_5, x_4, x_3, x_2 on the second row, x_6, x_5, x_4, x_3 on the third row, x_7, x_6, x_5, x_4 on the fourth row, and x_8, x_7, x_6, x_5 on the bottom row. The vector $\mathbf{w}$ contains elements w_1, w_2, w_3, w_4 . A brace next to $\mathbf{w}$ indicates the constraint $\|\mathbf{w}\|_0 \leq \tau$.

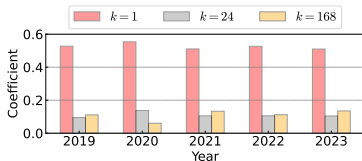
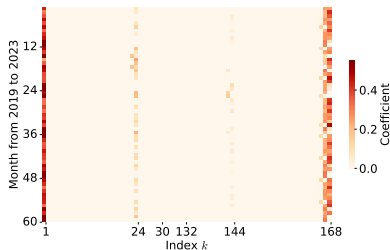
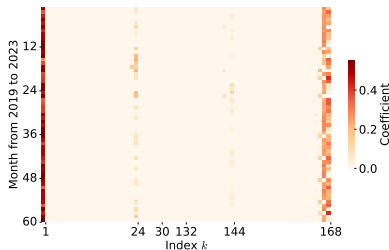
d th-order autoregression on time series $\mathbf{x} = (x_1, x_2, \dots, x_9)^\top$ w/ integer $\tau \in \mathbb{Z}^+$

- Sparse autoregression (Subspace Pursuit Algorithm (Dai & Milenkovic'09))

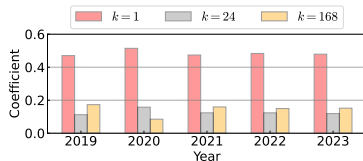
$$\begin{aligned} \min_{\mathbf{w} \geq 0} \quad & \|\tilde{\mathbf{x}} - \mathbf{A}\mathbf{w}\|_2^2 \\ \text{s.t.} \quad & \underbrace{\|\mathbf{w}\|_0}_{\text{Sparsity w/ } \ell_0\text{-norm}} \leq \tau \end{aligned}$$

Envisioning Human Mobility

- NYC rideshare: Sparse coefficient vectors across different months



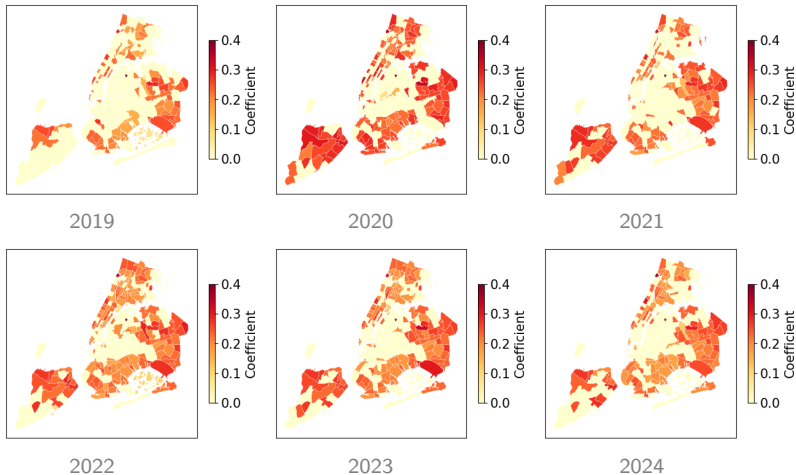
NYC pickup trips



NYC dropoff trips

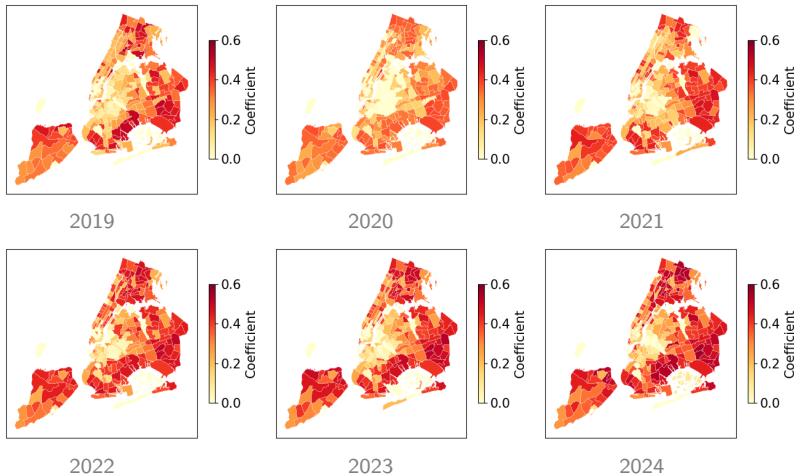
- Stronger daily periodicity vs. weaker weekly periodicity in 2020

Stronger Daily Periodicity in 2020



- High-demand areas are less periodic
- More areas show remarkable daily periodicity in 2020

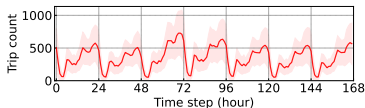
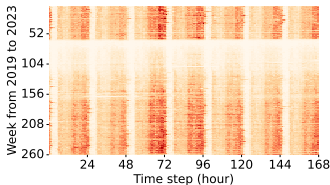
Weaker Weekly Periodicity in 2020



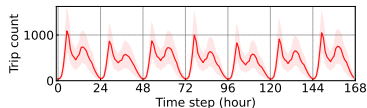
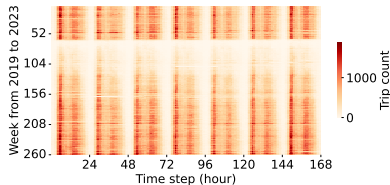
- High-demand areas are less periodic
- Less areas show remarkable weekly periodicity in 2020

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



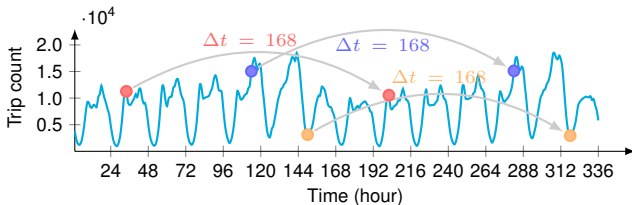
Dropoff trips

- Sparse coefficient vectors:

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

Solution Quality

- Subspace pursuit (SP) sometimes fails



Periodicity of rideshare trip time series

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

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

Time-Varying Transport Systems

- Rideshare trip data $\{\mathbf{x}_\gamma\}_{\gamma \in [\delta]}$ across $\gamma \in [\delta]$ months/years
- (Ours)** Reformulate interpretable sparse autoregression:

$$\begin{aligned} \min_{\{\mathbf{w}_\gamma\}_{\gamma \in [\delta]}} \quad & \sum_{\gamma \in [\delta]} \|\tilde{\mathbf{x}}_\gamma - \mathbf{A}_\gamma \mathbf{w}_\gamma\|_2^2 \\ \text{s.t.} \quad & \begin{cases} \mathbf{w}_\gamma \geq 0 & \text{(non-negativity)} \\ \|\mathbf{w}_\gamma\|_0 \leq \tau & \text{(sparsity)} \\ |\text{supp}(\mathbf{w}_\gamma) \cup \text{supp}(\mathbf{w}_{\gamma+1})| \\ \quad - |\text{supp}(\mathbf{w}_\gamma) \cap \text{supp}(\mathbf{w}_{\gamma+1})| = 0 & \text{(no local difference)} \end{cases} \end{aligned}$$

making $\text{supp}(\mathbf{w}_\gamma) = \text{supp}(\mathbf{w}_{\gamma+1})$ comparable across δ months/years.

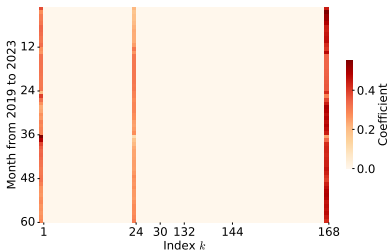
- Constraints w/ binary variables $\beta_\gamma \in \{0, 1\}^d$:

$$\underbrace{0 \leq \mathbf{w}_\gamma \leq \beta_\gamma}_{\text{upper bound } \{0, 1\}} \quad \underbrace{\sum_{k \in [d]} \beta_{\gamma, k} \leq \tau}_{\text{sum of binary var.}} \quad \underbrace{\beta_\gamma - \beta_{\gamma+1} = 0}_{\text{comparability across } \mathbf{w}_\gamma, \forall \gamma}$$

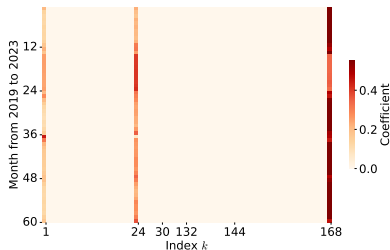
- MIP problem w/ $2d\delta$ decision variables!
- (Efficiency?)** ML prunes the search space, e.g., $2\tau_0\delta$ decision variables ($\tau < \tau_0 \ll d$) instead.

John F. Kennedy International Airport

- Coefficients $\{w_\gamma\}_{\gamma \in [\delta]}$ at $S = \{\underbrace{1}_{\text{local}}, \underbrace{24}_{\text{daily}}, \underbrace{168}_{\text{weekly}}\}$ across $\delta = 60$ months
 - ① Stronger weekly periodicity of dropoff trips than pickup trips
 - ② Stronger daily periodicity in 2020
 - ③ Weaker weekly periodicity in 2020



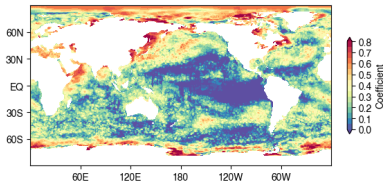
Pickup trips



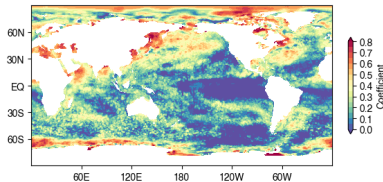
Dropoff trips

- Identify system patterns that evolve over time for human mobility

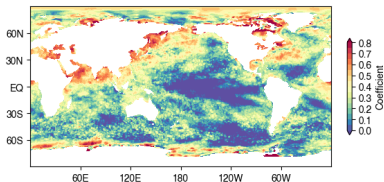
Beyond Transport: Sea Surface Temperature



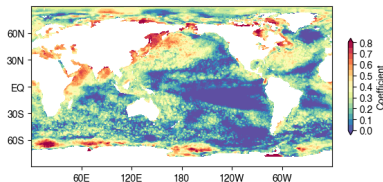
1980s



1990s



2000s



2010s

- Identify yearly periodicity at $k = 12$ from SST data ($\tau = 4$)
 - 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 change & global warming & sustainable development



Thanks for your attention!

 Technical University of Munich

Any Questions?

About me:

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