



# Machine Learning and Optimization for Data-Driven Transportation Analytics

Tensor Decomposition, Interpretable ML, Mathematical Programming

• School of Management, Technical University of Munich

**Xinyu Chen**

Postdoctoral Associate, MIT

December 6, 2024

# Transport Data

- Transport & mobility application scenarios



Highway (Portland)



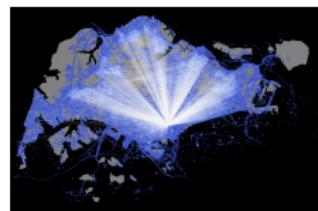
Uber movement (NYC)



Uber movement (Seattle)



Taxi trajectory (Shenzhen)



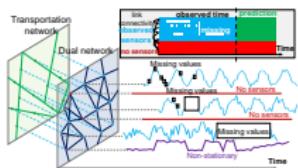
Human movement (Singapore)

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

# Data-Driven Transportation Analytics

## Part I

### Traffic Imputation

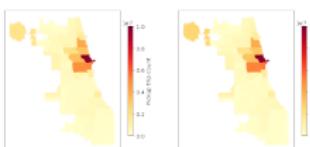


Chen et al.'24

Matrix/tensor completion  
Circulant matrix  
Circular convolution  
Fast Fourier transform

## Part II

### Pattern Discovery

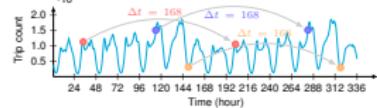


Chen et al.'24

Time series autoregression  
Tensor decomposition  
Conjugate gradient  
Procrustes problems

## Part III

### Periodicity Qualification



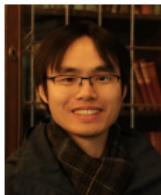
Working paper

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

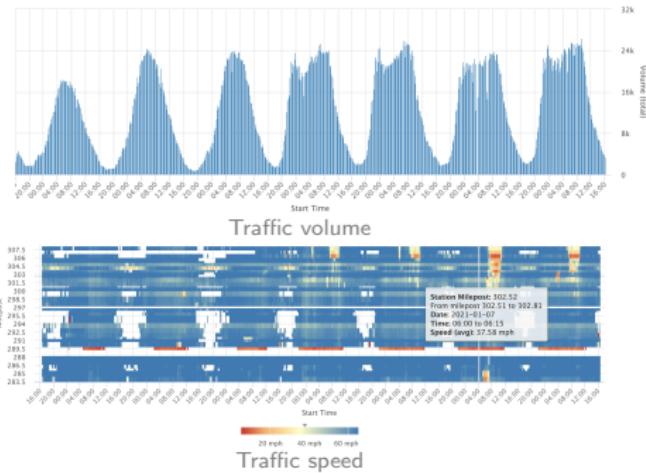


Lijun Sun  
McGill

- **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 data<sup>1</sup>



- $X \in \mathbb{R}^{N \times T}$  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?

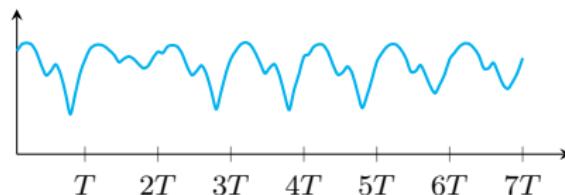
<sup>1</sup><https://portal.its.pdx.edu/home>

# Time Series Imputation

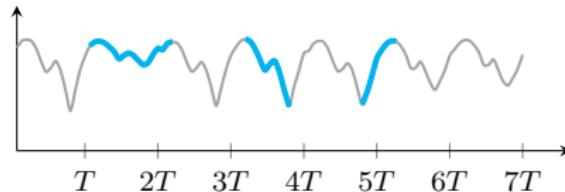
---

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

Undirected and circulant graph

Modeling →

$$\mathbf{L} = \begin{bmatrix} 2 & -1 & 0 & 0 & -1 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ -1 & 0 & 0 & -1 & 2 \end{bmatrix}$$

(Circulant) Laplacian matrix

- Laplacian kernel:

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

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

- Temporal regularization:

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

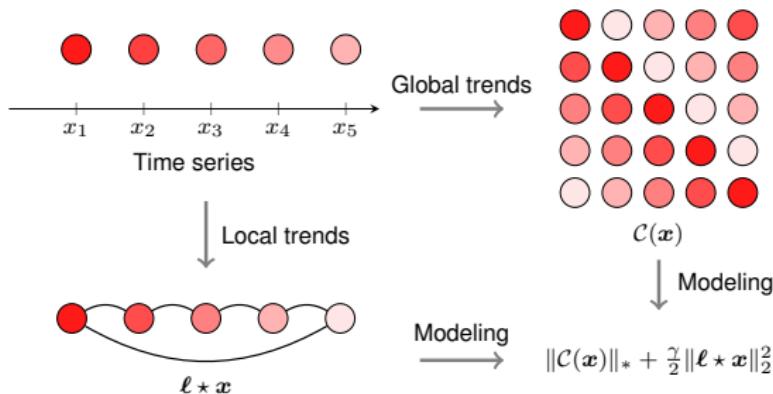
# Global + Local Trends?

## Laplacian Convolutional Representation (LCR)

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

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

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



# Laplacian Convolutional Representation

- Augmented Lagrangian function:<sup>2</sup>

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

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

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

- Reformulate the optimization as  $\ell_1$ -norm minimization:

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

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

---

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

# Laplacian Convolutional Representation

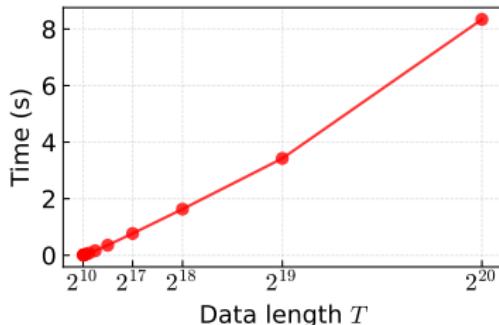
$\ell_1$ -norm Minimization (Liu & Zhang'23)

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

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

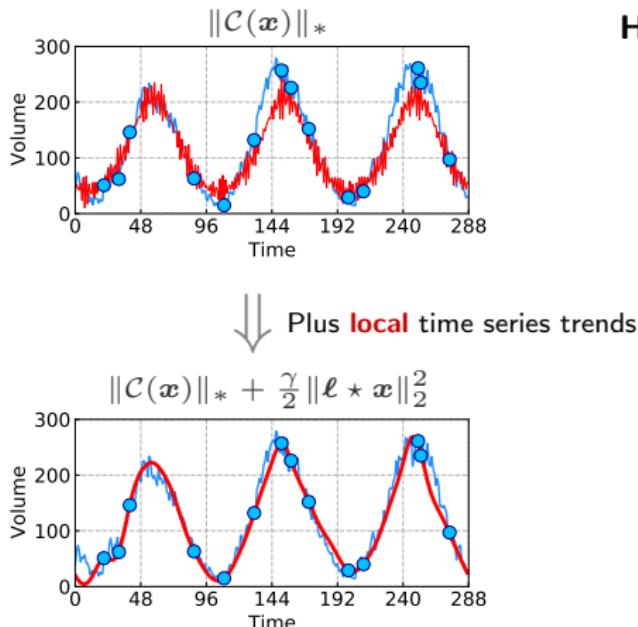
$$\hat{x}_t := \frac{\hat{h}_t}{|\hat{h}_t|} \cdot \underbrace{\max\{0, |\hat{h}_t| - 1/\delta\}}_{\text{shrinkage (e.g., ReLU)}}, t \in [T].$$

- **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 imputation<sup>3</sup> (95% missing rate)



## 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:

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

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

<sup>3</sup>Blue dot: partial observation; red line: imputation.

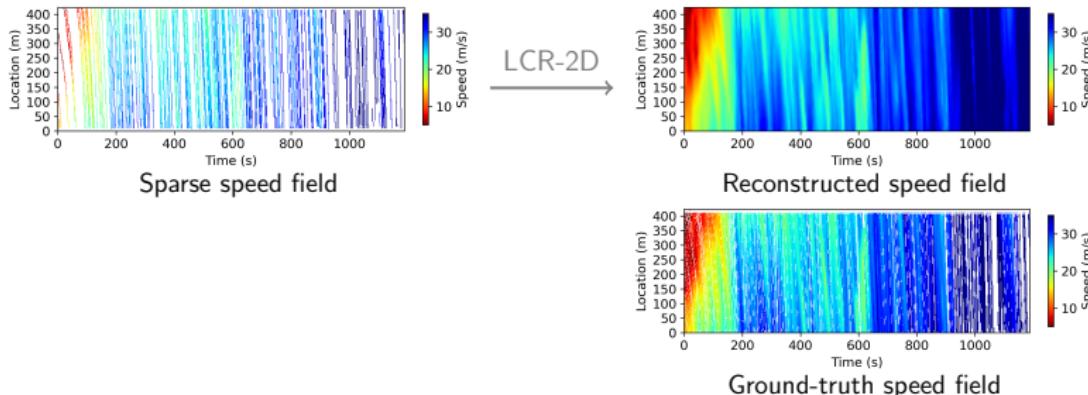
# Experiments

Speed field reconstruction in German highways<sup>4</sup>

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

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

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



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

# Discovering Dynamic Patterns from Spatiotemporal Systems



Xinyu Chen  
UdeM → MIT



Nicolas Saunier  
PolyMtl



Lijun Sun  
McGill



Dingyi Zhuang  
MIT



HanQin Cai  
UCF



Shenhao Wang  
UF

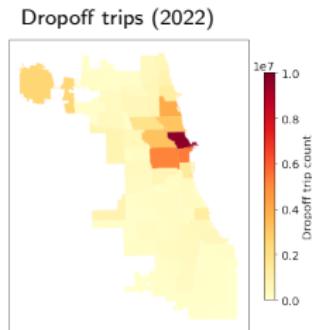
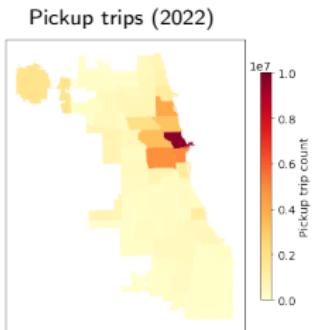
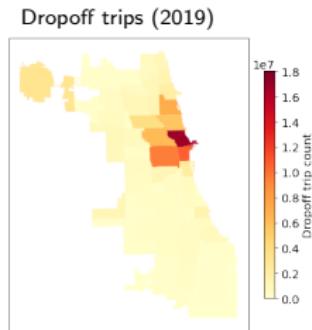
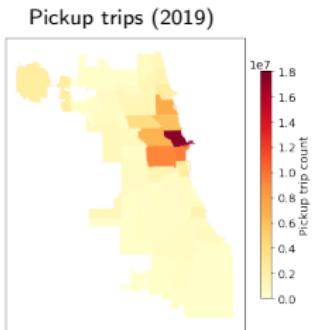


Jinhua Zhao  
MIT

- **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

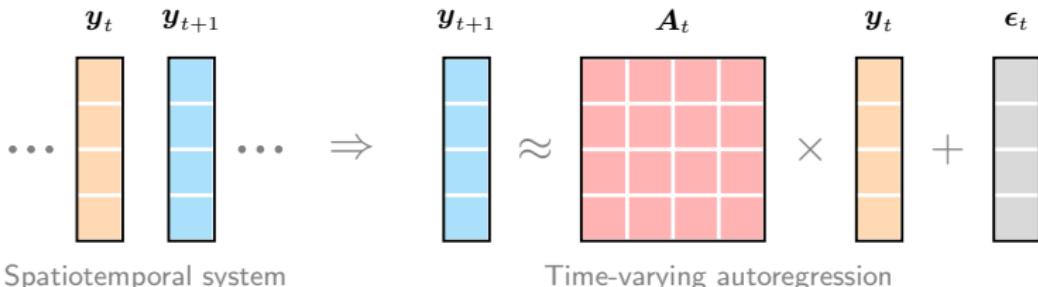
- Chicago rideshare: 96.6M trips (2019) vs. 57.3M trips (2022)



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

# Autoregression

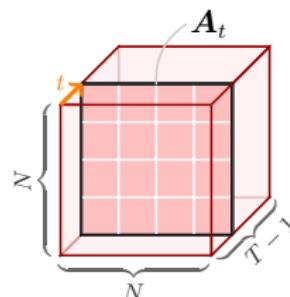
- How to characterize dynamical systems?

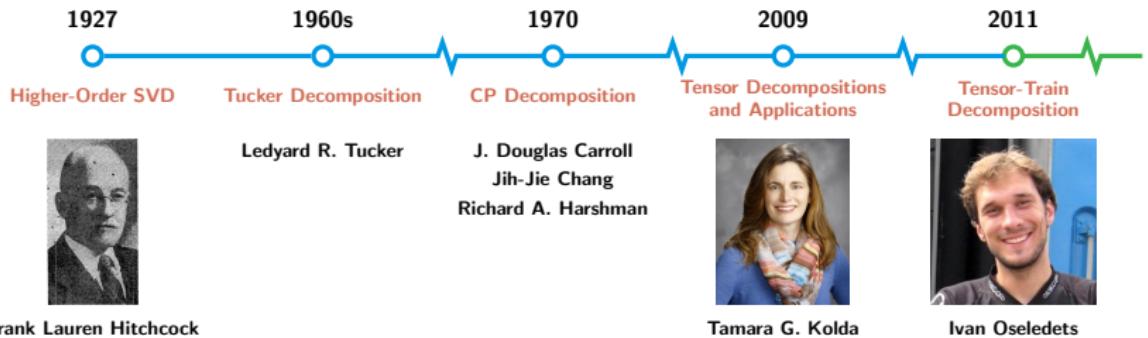


- On spatiotemporal data  $\mathbf{Y} \in \mathbb{R}^{N \times T}$ :

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

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

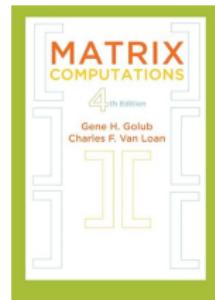




# Dynamic Autoregressive Tensor Factorization

- Tensor factorization:

$$\mathcal{A} = \underbrace{\mathcal{G} \times_1 \mathbf{W} \times_2 \mathbf{V} \times_3 \mathbf{X}}_{\text{Tucker decomposition}}$$
$$\Downarrow$$
$$\mathbf{A}_t = \mathcal{G} \times_1 \underbrace{\mathbf{W}}_{\text{spatial modes}} \times_2 \mathbf{V} \times_3 \underbrace{\mathbf{x}_t^\top}_{\text{temporal modes}}$$



- Optimization problem:

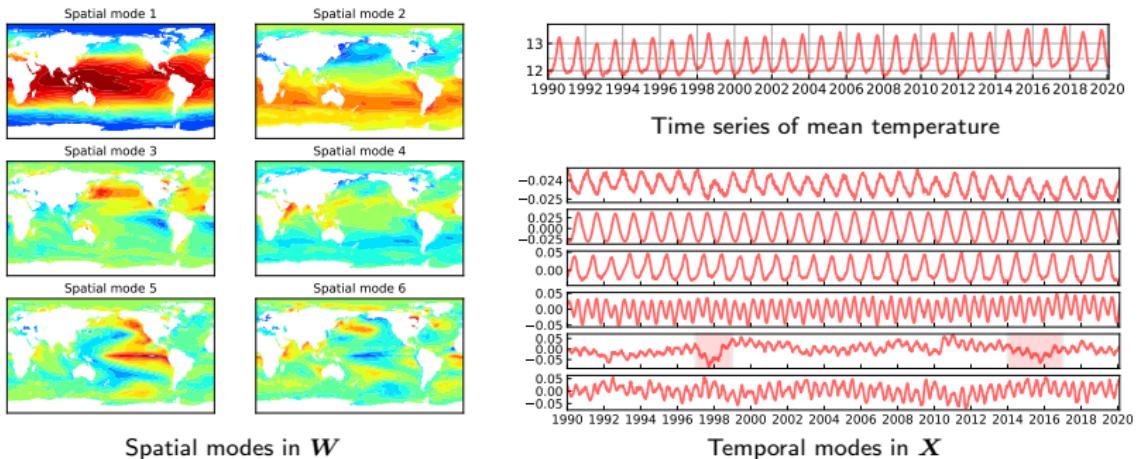
$$\min_{\mathcal{G}, \mathbf{W}, \mathbf{V}, \mathbf{X}} \frac{1}{2} \sum_{t \in [T-1]} \| \mathbf{y}_{t+1} - (\mathcal{G} \times_1 \mathbf{W} \times_2 \mathbf{V} \times_3 \mathbf{x}_t^\top) \mathbf{y}_t \|_2^2$$

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

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

# Beyond Transport: Sea Surface Temperature

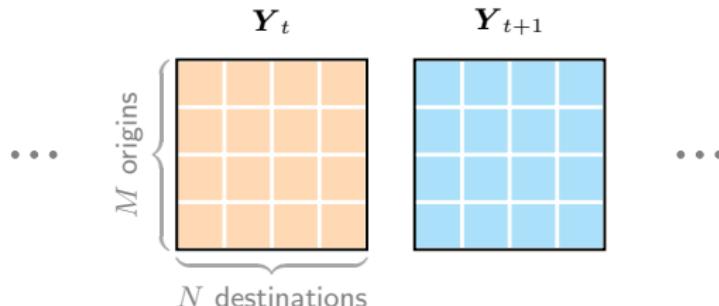
- Sea surface temperature (**SST**) dataset



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

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

- Optimization problem:

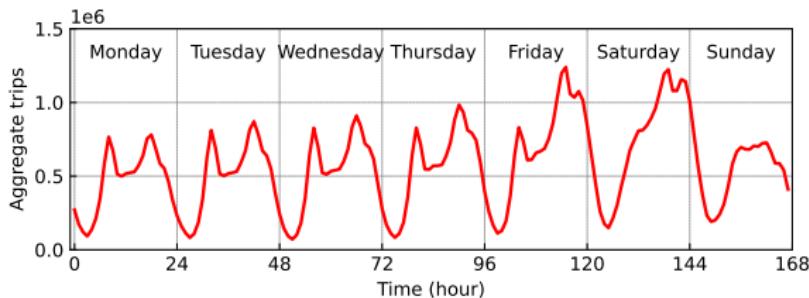
$$\min_{\mathcal{G}, \mathbf{W}, \mathbf{U}, \mathbf{V}, \mathbf{x}} \frac{1}{2} \sum_{n \in [N]} \sum_{t \in [T-1]} \left\| \mathbf{y}_{n,t+1} - \underbrace{(\mathcal{G} \times_1 \mathbf{W} \times_2 \mathbf{U} \times_3 \mathbf{V} \times_4 \mathbf{x}_t^\top) \mathbf{y}_{n,t}}_{\text{Tucker decomposition}}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

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

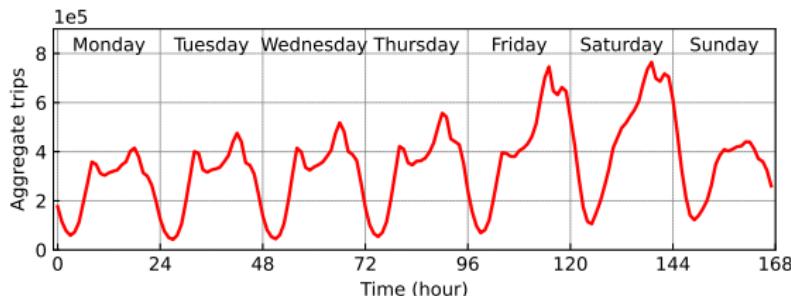
# Human Mobility

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

Pickup trips aggregated over 52 weeks in 2019

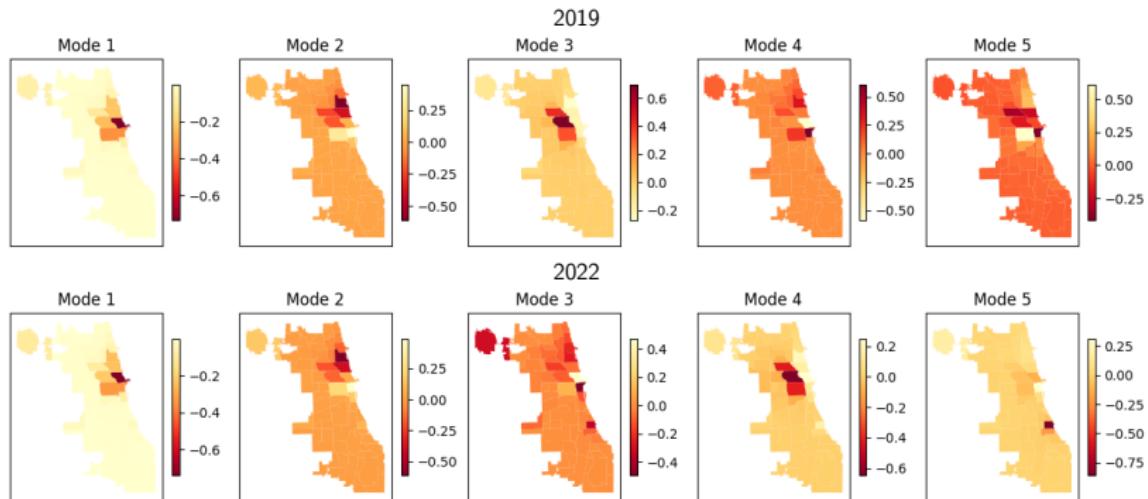


Pickup trips aggregated over 52 weeks in 2022



# Human Mobility

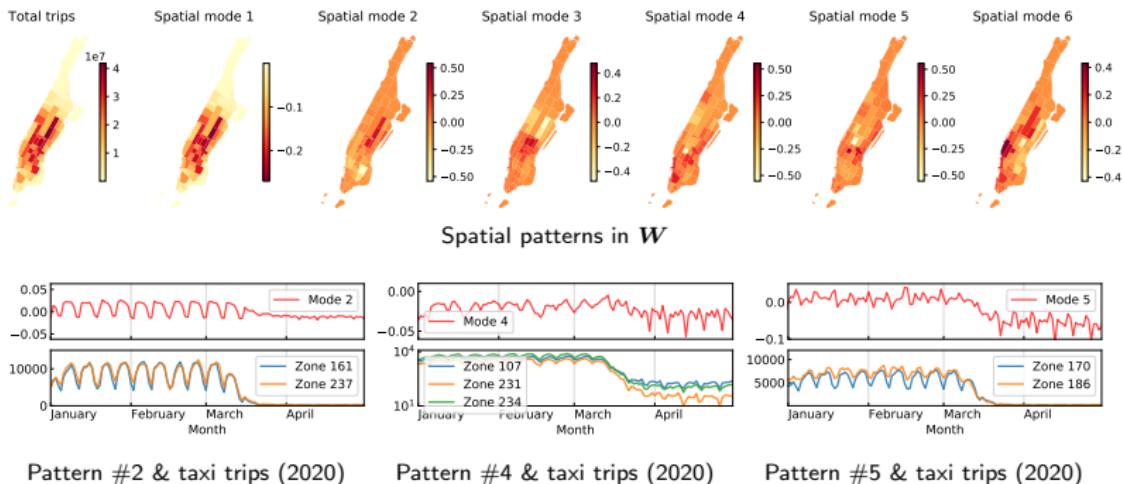
- Rideshare trip data: 77 origins  $\times$  77 destinations  $\times$  168 hours



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

# Human Mobility

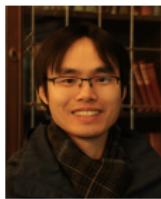
- NYC taxi dataset (pickup)
  - Remarkable decrease of trips due to COVID-19



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

# Quantifying Periodicity of Human Mobility

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



Xinyu Chen  
MIT DUSP



Vassilis Digalakis Jr  
BU Business



Lijun Ding  
UCSD Math



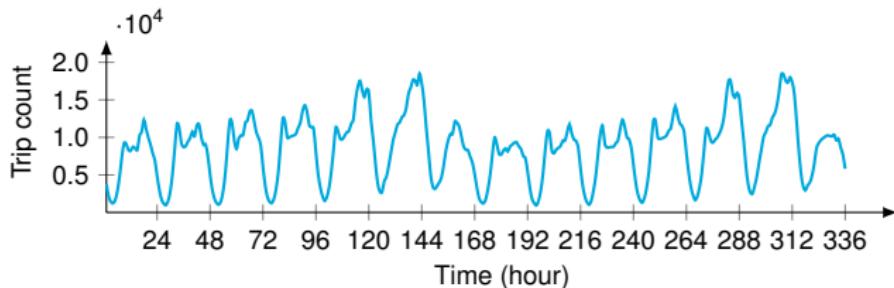
Dingyi Zhuang  
MIT CEE



Jinhua Zhao  
MIT DUSP

# Motivation

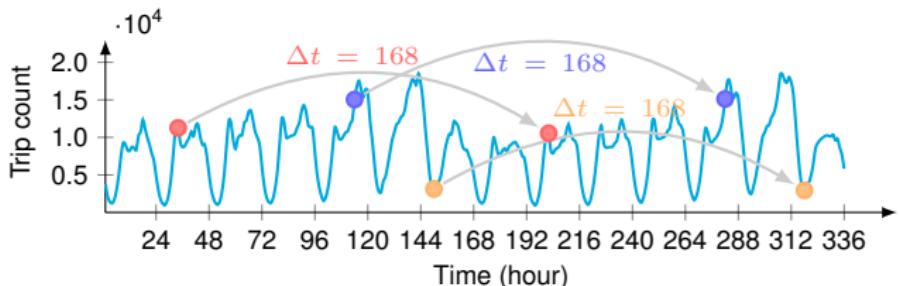
---



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

# Motivation

---



Weekly periodicity of rideshare trip time series

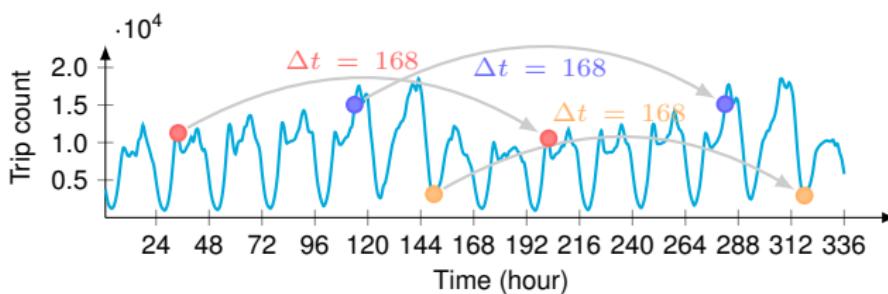
What motivates us most about **periodicity**?

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

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



Periodicity of rideshare trip time series

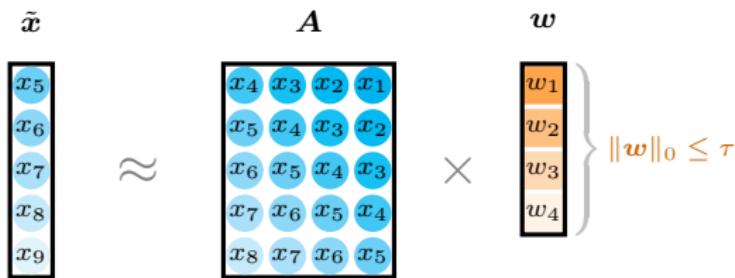
- Sparse coefficient vector  $\mapsto$  **Interpretability?**

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

# Valorizing Autoregression

- Time series autoregression

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



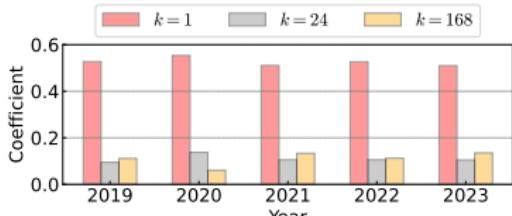
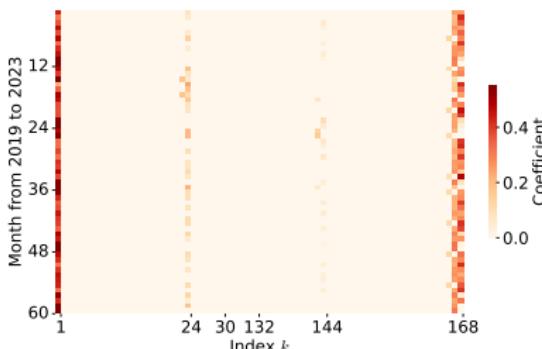
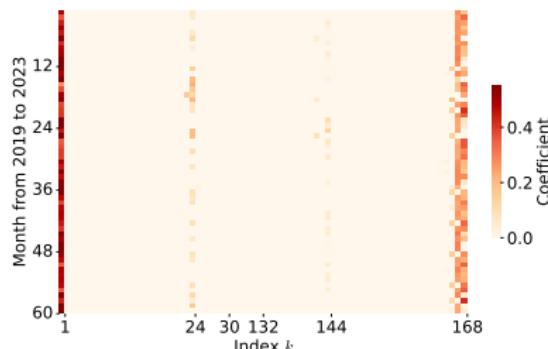
dth-order autoregression on time series  $\mathbf{x} = (x_1, x_2, \dots, x_9)^\top$  w/ integer  $\tau \in \mathbb{Z}^+$

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

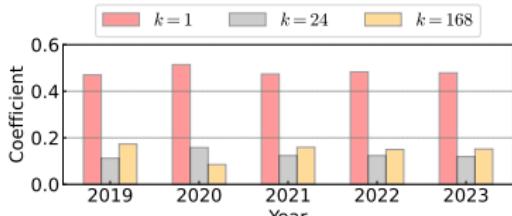
$$\begin{aligned} \min_{\mathbf{w} \geq 0} \quad & \| \tilde{\mathbf{x}} - \mathbf{A}\mathbf{w} \|_2^2 \\ \text{s.t.} \quad & \underbrace{\|\mathbf{w}\|_0 \leq \tau}_{\text{Sparsity w/ } \ell_0\text{-norm}} \end{aligned}$$

# Envisioning Human Mobility

- NYC rideshare: Sparse coefficient vectors across different months



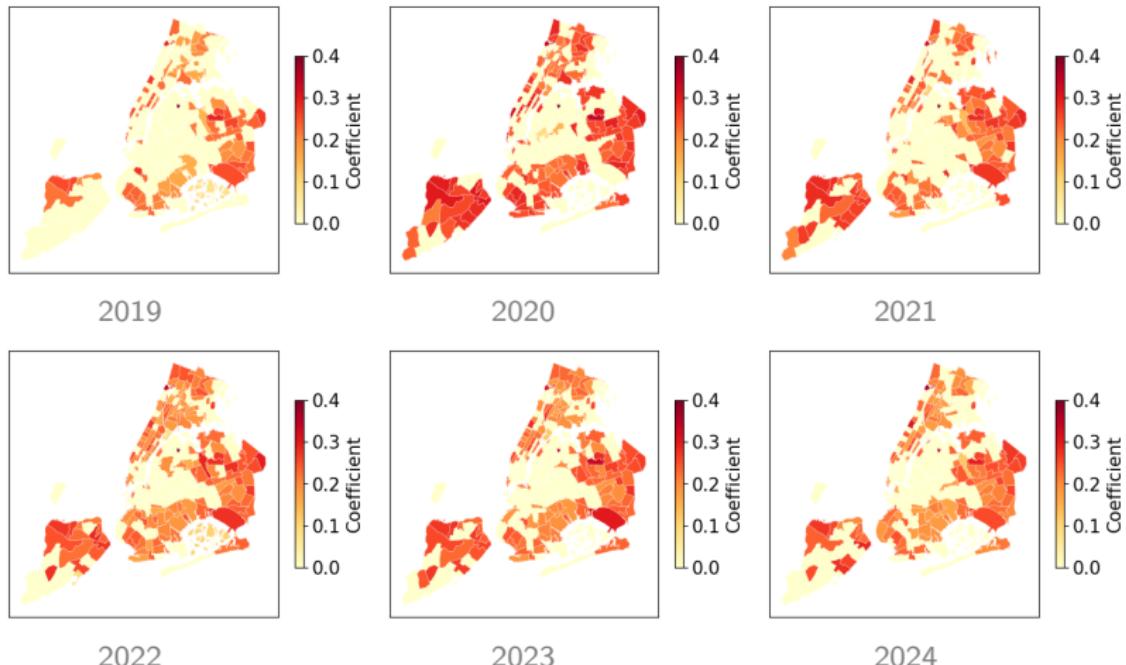
NYC pickup trips



NYC dropoff trips

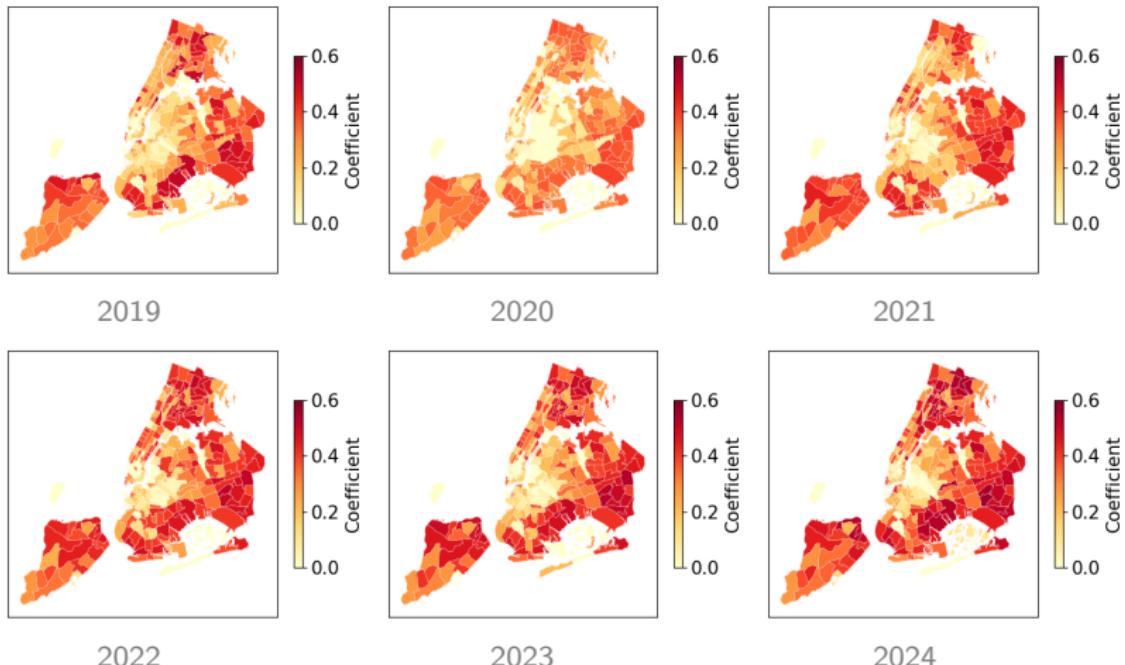
- Stronger daily periodicity vs. weaker weekly periodicity in 2020

# Stronger Daily Periodicity in 2020



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

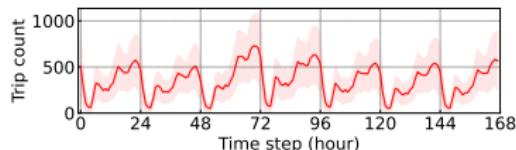
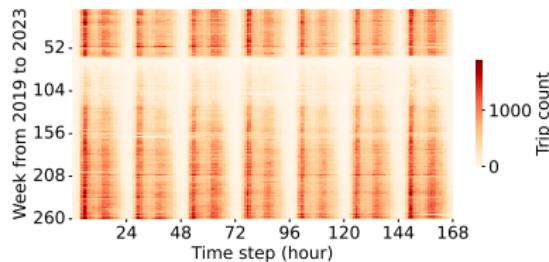
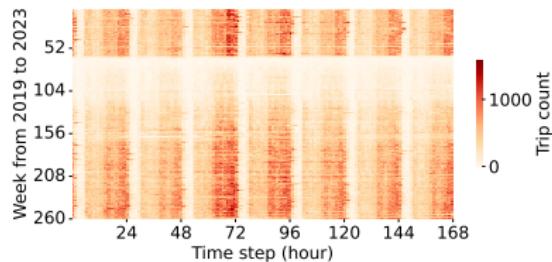
## Weaker Weekly Periodicity in 2020



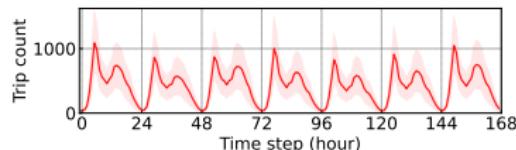
- High-demand areas are less periodic
- Less areas show remarkable weekly periodicity in 2020

# 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



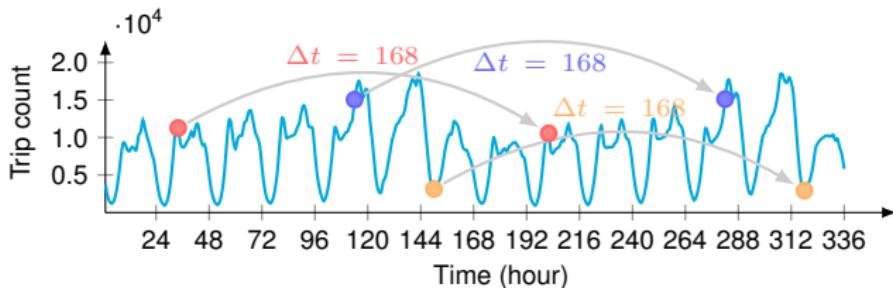
Dropoff trips

- 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  $\tau = 2$ ):

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

# Time-Varying Transport Systems

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

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

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

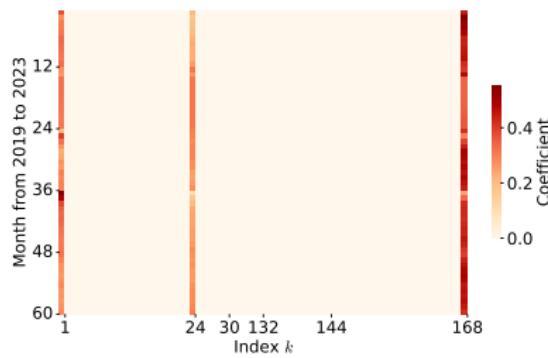
- Constraints w/ binary variables  $\beta_\gamma \in \{0, 1\}^d$ :

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

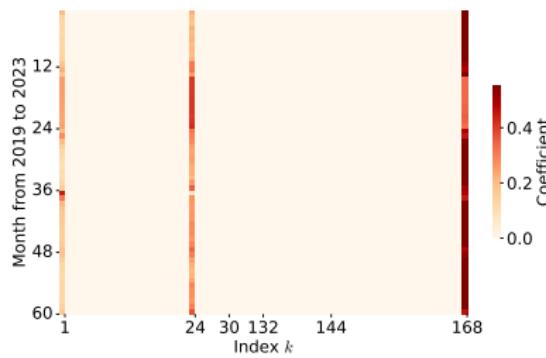
- MIP problem w/  $2d\delta$  decision variables!
- **(Efficiency?)** ML prunes the search space, e.g.,  $2\tau_0\delta$  decision variables ( $\tau < \tau_0 \ll d$ ) instead.

# 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



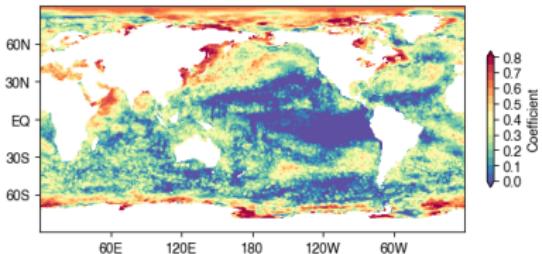
Pickup trips



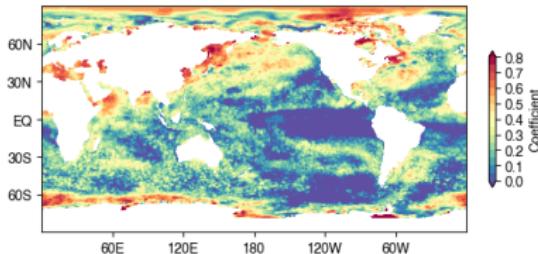
Dropoff trips

- Identify system patterns that evolve over time for human mobility

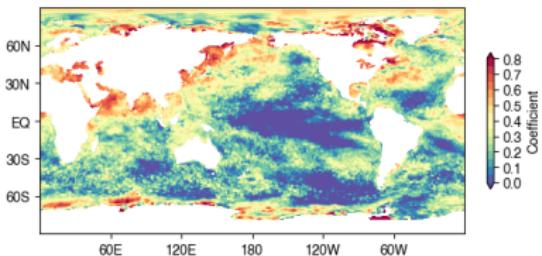
# Beyond Transport: Sea Surface Temperature



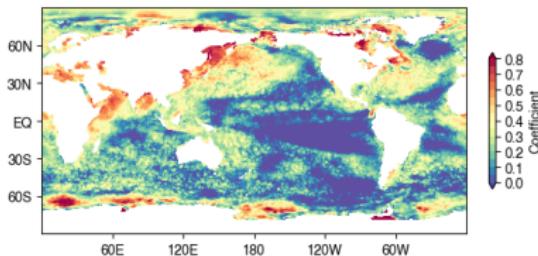
1980s



1990s



2000s



2010s

- Identify yearly periodicity at  $k = 12$  from SST data ( $\tau = 4$ )
  - The areas of El Nino events are less seasonal/predictable
  - 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:

- 🏠 Homepage: <https://xinychen.github.io>
- 🏠 MIT sites: <https://sites.mit.edu/xinychen>
- ✉ How to reach me: [xinychen@mit.edu](mailto:xinychen@mit.edu)