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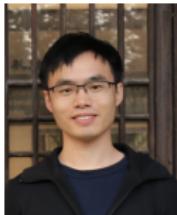


# Nonstationary Temporal Matrix Factorization for Multivariate Time Series Forecasting

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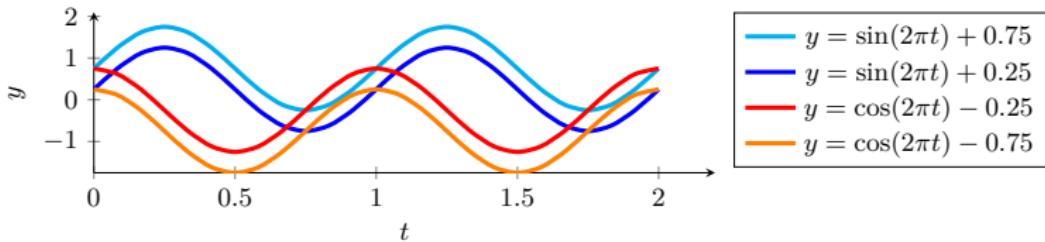
## Source

- ❶ **Preprint:** Xinyu Chen, Chengyuan Zhang, Xi-Le Zhao, Nicolas Saunier, Lijun Sun (2022). Nonstationary temporal matrix factorization for multivariate time series forecasting. arXiv preprint arXiv:2203.10651.
- ❷ **Data & Python code:** <https://github.com/xinyuchen/tracebase>
- ❸ **Blog post:** <https://medium.com/@xinyu.chen>
- ❹ **Slides:** <https://xinyuchen.github.io/slides/notmf.pdf>

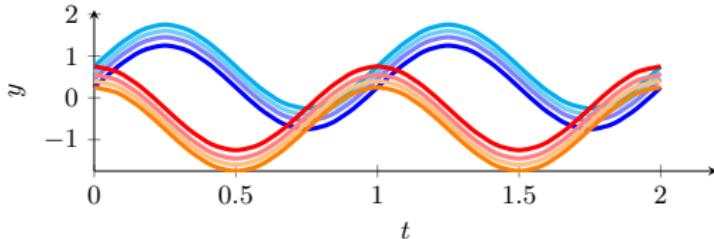
# Motivation

**[M1]** High-dimensional time series could stem from a relatively small number of latent temporal factors.

- Four sequences with two kinds of temporal dynamics (Sine & Cosine).



- Several sequences with two kinds of temporal dynamics.



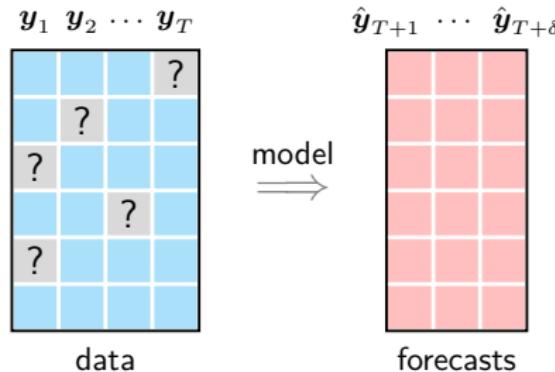
**[M2]** Sparse time series may reveal low-rank patterns.

**[M3]** Modern time series usually show nonstationarity (e.g., trend, seasonality).

# Objective

## Multivariate time series forecasting

- Given a partially observed data  $\mathbf{Y} \in \mathbb{R}^{N \times T}$  consisting of time series  $\mathbf{y}_1, \dots, \mathbf{y}_T \in \mathbb{R}^N$ , forecast data points  $\hat{\mathbf{y}}_{T+\delta}, \delta \in \mathbb{N}^+$ .



[Q]

- How to learn from *high-dimensional* and *sparse* data?
- How to model *nonstationarity* in time series?
- How to perform forecasting on these time series?

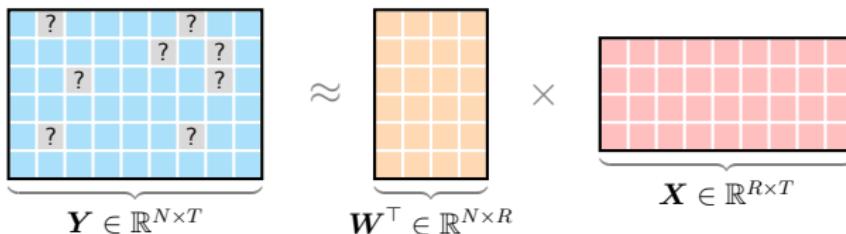
# Methodology

## Low-rank matrix factorization (Koren et al.'09)

Given any partially observed data matrix  $\mathbf{Y} \in \mathbb{R}^{N \times T}$  with observed index set  $\Omega$ , then the optimization problem of matrix factorization with rank  $R$  can be formulated as

$$\min_{\mathbf{W}, \mathbf{X}} \frac{1}{2} \|\mathcal{P}_\Omega(\mathbf{Y} - \mathbf{W}^\top \mathbf{X})\|_F^2 + \frac{\rho}{2} (\|\mathbf{W}\|_F^2 + \|\mathbf{X}\|_F^2) \quad (1)$$

- :( Cannot capture temporal correlations.
- :( Cannot perform time series forecasting.



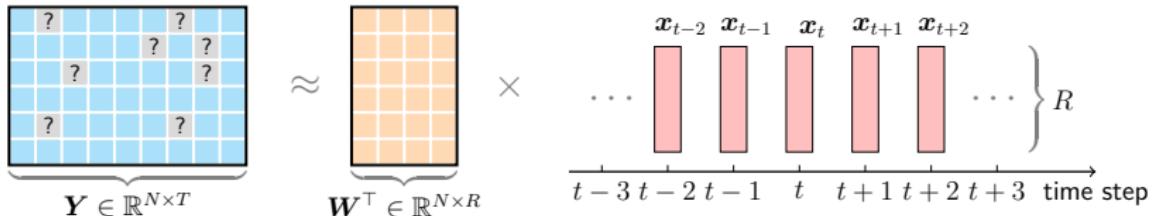
# Methodology

## Temporal matrix factorization (Yu et al.'16; Chen & Sun'21)

Given any partially observed time series data  $\mathbf{Y} \in \mathbb{R}^{N \times T}$  with observed index set  $\Omega$ , then temporal matrix factorization assumes a  $d$ th-order vector autoregressive (VAR) process on the temporal factor matrix:

$$\begin{aligned} \min_{\mathbf{W}, \mathbf{X}, \{\mathbf{A}_k\}_{k=1}^d} \quad & \frac{1}{2} \|\mathcal{P}_\Omega(\mathbf{Y} - \mathbf{W}^\top \mathbf{X})\|_F^2 + \frac{\rho}{2} (\|\mathbf{W}\|_F^2 + \|\mathbf{X}\|_F^2) \\ & + \frac{\lambda}{2} \sum_{t=d+1}^T \|\mathbf{x}_t - \sum_{k=1}^d \mathbf{A}_k \mathbf{x}_{t-k}\|_2^2 \end{aligned} \tag{2}$$

 VAR is usually built on stationary time series (temporal factors).



# Methodology

## Nonstationary temporal matrix factorization (NoTMF)

Given any partially observed time series data  $\mathbf{Y} \in \mathbb{R}^{N \times T}$  with observed index set  $\Omega$ , then we assume a season- $m$  differencing on the latent temporal factors:

$$\begin{aligned} \min_{\mathbf{W}, \mathbf{X}, \{\mathbf{A}_k\}_{k=1}^d} & \frac{1}{2} \|\mathcal{P}_\Omega(\mathbf{Y}) - \mathcal{P}_\Omega(\mathbf{W}^\top \mathbf{X})\|_F^2 + \frac{\rho}{2} (\|\mathbf{W}\|_F^2 + \|\mathbf{X}\|_F^2) \\ & + \frac{\lambda}{2} \sum_{t=d+m+1}^T \|(\mathbf{x}_t - \mathbf{x}_{t-m}) - \sum_{k=1}^d \mathbf{A}_k (\mathbf{x}_{t-k} - \mathbf{x}_{t-m-k})\|_2^2 \end{aligned} \quad (3)$$

- First-order differencing  $\mathbf{x}'_t = \mathbf{x}_t - \mathbf{x}_{t-1}$ .
  - Second-order differencing  $\mathbf{x}''_t = (\mathbf{x}_t - \mathbf{x}_{t-1}) - (\mathbf{x}_{t-1} - \mathbf{x}_{t-2})$ .
  - Twice-differenced series  $\mathbf{x}'''_t = (\mathbf{x}_t - \mathbf{x}_{t-m}) - (\mathbf{x}_{t-1} - \mathbf{x}_{t-m-1})$ .
- 😊 Stationarizing a time series with differencing can improve the prediction.<sup>1</sup>

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<sup>1</sup>Stationarity and differencing: <https://otexts.com/fpp2/stationarity.html>

# Methodology

Rewrite VAR in the form of matrix

## Temporal operators

For any multivariate time series  $\mathbf{X} \in \mathbb{R}^{R \times T}$  with  $m, d \in \mathbb{N}^+$ , if we define temporal operators as

$$\begin{aligned}\Psi_k &\triangleq \begin{bmatrix} \mathbf{0}_{(T-d-m) \times (d-k)} & -\mathbf{I}_{T-d-m} & \mathbf{0}_{(T-d-m) \times (k+m)} \end{bmatrix} \\ &+ \begin{bmatrix} \mathbf{0}_{(T-d-m) \times (d+m-k)} & \mathbf{I}_{T-d-m} & \mathbf{0}_{(T-d-m) \times k} \end{bmatrix} \\ &\in \mathbb{R}^{(T-d-m) \times T}, \quad k = 0, 1, \dots, d\end{aligned}\tag{4}$$

then

$$\begin{aligned}&\sum_{t=d+m+1}^T \|(\mathbf{x}_t - \mathbf{x}_{t-m}) - \sum_{k=1}^d \mathbf{A}_k (\mathbf{x}_{t-k} - \mathbf{x}_{t-m-k})\|_2^2 \\ &\equiv \|\mathbf{X}\Psi_0^\top - \sum_{k=1}^d \mathbf{A}_k \mathbf{X}\Psi_k^\top\|_F^2 \triangleq \|\mathbf{X}\Psi_0^\top - \mathbf{A}(\mathbf{I}_d \otimes \mathbf{X})\Psi^\top\|_F^2\end{aligned}\tag{5}$$

where  $\mathbf{A} \triangleq [\mathbf{A}_1 \quad \cdots \quad \mathbf{A}_d]$  and  $\Psi \triangleq [\Psi_1 \quad \cdots \quad \Psi_d]$ .

# Methodology

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Rewrite NoTMF:

$$\begin{aligned} \min_{\mathbf{W}, \mathbf{X}, \mathbf{A}} \quad & \frac{1}{2} \|\mathcal{P}_\Omega(\mathbf{Y} - \mathbf{W}^\top \mathbf{X})\|_F^2 + \frac{\rho}{2} (\|\mathbf{W}\|_F^2 + \|\mathbf{X}\|_F^2) \\ & + \frac{\lambda}{2} \|\mathbf{X} \Psi_0^\top - \mathbf{A} (\mathbf{I}_d \otimes \mathbf{X}) \Psi^\top\|_F^2 \end{aligned} \tag{6}$$

Alternating minimization method:

- w.r.t.  $\mathbf{W}$ :

$$\frac{\partial f}{\partial \mathbf{W}} = -\mathbf{X} \mathcal{P}_\Omega^\top (\mathbf{Y} - \mathbf{W}^\top \mathbf{X}) + \rho \mathbf{W} = \mathbf{0} \tag{7}$$

- w.r.t.  $\mathbf{X}$ :

$$\frac{\partial f}{\partial \mathbf{X}} = -\mathbf{W} \mathcal{P}_\Omega (\mathbf{Y} - \mathbf{W}^\top \mathbf{X}) + \rho \mathbf{X} + \lambda \sum_{k=0}^d \mathbf{A}_k^\top \left( \sum_{h=0}^d \mathbf{A}_h \mathbf{X} \Psi_h^\top \right) \Psi_k = \mathbf{0} \tag{8}$$

- w.r.t.  $\mathbf{A}$ :

$$\mathbf{A} = \mathbf{X} \Psi_0^\top [(\mathbf{I}_d \otimes \mathbf{X}) \Psi^\top]^\dagger \tag{9}$$

# Methodology

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Solve generalized Sylvester equation (w.r.t.  $\mathbf{X}$ ):

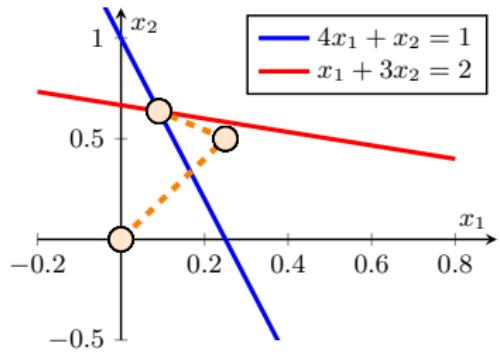
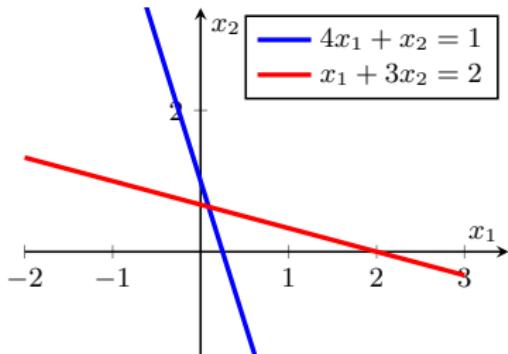
$$\underbrace{\mathbf{W}\mathcal{P}_\Omega(\mathbf{W}^\top \mathbf{X}) + \rho \mathbf{X} + \lambda \sum_{k=0}^d \mathbf{A}_k^\top \left( \sum_{h=0}^d \mathbf{A}_h \mathbf{X} \boldsymbol{\Psi}_h^\top \right) \boldsymbol{\Psi}_k}_{\mathcal{L}_x(\mathbf{X}) \triangleq \text{vec}(\cdot)} = \mathbf{W}\mathcal{P}_\Omega(\mathbf{Y})$$

- Conjugate gradient for inferring  $\mathbf{X}$ :

- Initialize  $\mathbf{x}$  as  $\mathbf{x}_0$ , and compute the residual  
 $r_0 := \text{vec}(\mathbf{W}\mathcal{P}_\Omega(\mathbf{Y})) - \mathcal{L}_x(\mathbf{X}_0)$ . Let  $\mathbf{q}_0 := \mathbf{r}_0$ .
- Repeat:
  - Convert  $\mathbf{q}_\ell$  into matrix  $\mathbf{Q}_\ell$ .
  - Compute  $\alpha_\ell := \frac{\mathbf{r}_\ell^\top \mathbf{r}_\ell}{\mathbf{q}_\ell^\top \mathcal{L}_x(\mathbf{Q}_\ell)}$ , and update
$$\begin{cases} \mathbf{x}_{\ell+1} := \mathbf{x}_\ell + \alpha_\ell \mathbf{q}_\ell \\ \mathbf{r}_{\ell+1} := \mathbf{r}_\ell - \alpha_\ell \mathcal{L}_x(\mathbf{Q}_\ell) \end{cases}.$$
  - Compute  $\beta_\ell := \frac{\mathbf{r}_{\ell+1}^\top \mathbf{r}_{\ell+1}}{\mathbf{r}_\ell^\top \mathbf{r}_\ell}$ , and update  $\mathbf{q}_{\ell+1} := \mathbf{r}_{\ell+1} + \beta_\ell \mathbf{q}_\ell$ .
  - Update  $\ell := \ell + 1$ .

# Methodology

- [Q]  $Ax = b$  with known  $A \in \mathbb{R}^n, b \in \mathbb{R}^n$ , the solution of  $x \in \mathbb{R}^n$ ?
- **Conjugate gradient** method:
  - o Initialize  $x$  as  $x_0$ , and compute the residual  $r_0 := b - Ax_0$ . Let  $q_0 := r_0$ .
  - o Repeat:
    - o Compute  $\alpha_\ell := \frac{r_\ell^\top r_\ell}{q_\ell^\top A q_\ell}$ , and update  $\begin{cases} x_{\ell+1} := x_\ell + \alpha_\ell q_\ell \\ r_{\ell+1} := r_\ell - \alpha_\ell A q_\ell \end{cases}$ .
    - o Compute  $\beta_\ell := \frac{r_{\ell+1}^\top r_{\ell+1}}{r_\ell^\top r_\ell}$ , and update  $q_{\ell+1} := r_{\ell+1} + \beta_\ell q_\ell$ .
    - o Update  $\ell := \ell + 1$ .



# Forecasting

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$$\underbrace{\mathbf{Y}_t \in \mathbb{R}^{N \times t}}_{\text{Matrix } \mathbf{Y}_t}$$

A 4x5 matrix  $\mathbf{Y}_t$  with the last column colored red. The first four columns have question marks in their top-right corners, indicating they are known past observations. The last column has question marks in its middle cells, indicating it is a future forecast.

$$R \left\{ \begin{array}{ccccccccc} \mathbf{x}_{t-3} & \mathbf{x}_{t-2} & \mathbf{x}_{t-1} & \mathbf{x}_t & \mathbf{x}_{t+1} \\ \hline t-3 & t-2 & t-1 & t & t+1 & t+2 & t+3 & \text{time step} \end{array} \right. \hat{\mathbf{x}}_{t+1} = \mathbf{x}_{t+1-m} + \text{VAR}(d, m)$$

A sequence of vectors  $\mathbf{x}_{t-3}, \mathbf{x}_{t-2}, \mathbf{x}_{t-1}, \mathbf{x}_t, \mathbf{x}_{t+1}$  corresponding to time steps  $t-3, t-2, t-1, t, t+1$ . The vector  $\mathbf{x}_{t+1}$  is highlighted in red and labeled  $x_{t+1}$ . A red bracket labeled  $R$  groups the vectors from  $t-3$  to  $t+1$ . A horizontal arrow below the  $x$  labels indicates the time step from  $t-3$  to  $t+3$ . The equation  $\hat{\mathbf{x}}_{t+1} = \mathbf{x}_{t+1-m} + \text{VAR}(d, m)$  is shown.

$$\underbrace{\mathbf{Y}_{t+1} \in \mathbb{R}^{N \times (t+1)}}_{\text{Matrix } \mathbf{Y}_{t+1}}$$

A 4x6 matrix  $\mathbf{Y}_{t+1}$  with the last column colored red. The first five columns have question marks in their top-right corners, indicating they are known past observations. The last column has question marks in its middle cells, indicating it is a future forecast.

$$R \left\{ \begin{array}{ccccccccc} \mathbf{x}_{t-3} & \mathbf{x}_{t-2} & \mathbf{x}_{t-1} & \mathbf{x}_t & \mathbf{x}_{t+1} & \mathbf{x}_{t+2} \\ \hline t-3 & t-2 & t-1 & t & t+1 & t+2 & t+3 & \text{time step} \end{array} \right. \hat{\mathbf{x}}_{t+2} = \mathbf{x}_{t+2-m} + \text{VAR}(d, m)$$

A sequence of vectors  $\mathbf{x}_{t-3}, \mathbf{x}_{t-2}, \mathbf{x}_{t-1}, \mathbf{x}_t, \mathbf{x}_{t+1}, \mathbf{x}_{t+2}$  corresponding to time steps  $t-3, t-2, t-1, t, t+1, t+2$ . The vectors from  $t$  to  $t+2$  are highlighted in orange, while the vector  $\mathbf{x}_{t+3}$  is highlighted in red and labeled  $x_{t+2}$ . A red bracket labeled  $R$  groups the vectors from  $t-3$  to  $t+2$ . A horizontal arrow below the  $x$  labels indicates the time step from  $t-3$  to  $t+3$ . The equation  $\hat{\mathbf{x}}_{t+2} = \mathbf{x}_{t+2-m} + \text{VAR}(d, m)$  is shown.

# Uber Movement Data

## High-dimensionality & Sparsity

- Uber (hourly) movement speed data<sup>2</sup>



NYC movement



Seattle movement

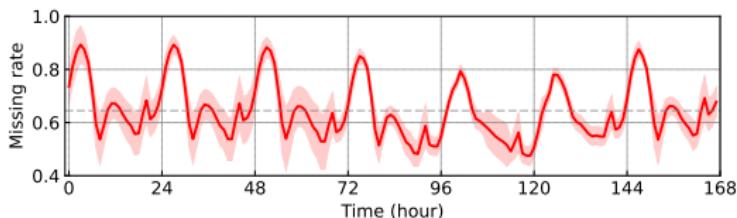
- The average speed on a given road segment for each hour of each day.
- Hourly speeds are computed when road segments have 5+ unique trips.
- **Issue:** insufficient sampling of ridesharing vehicles on the road network.

<sup>2</sup><https://movement.uber.com/>

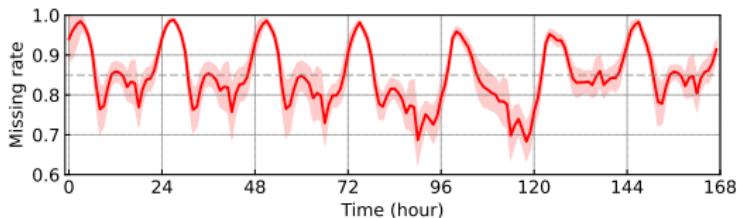
# Uber Movement Data

## High-dimensionality & Sparsity

- **NYC** movement speed data (2019)
  - **98,210** road segments & 8,760 time steps (hours)
  - Whole missing rate: **64.43%**

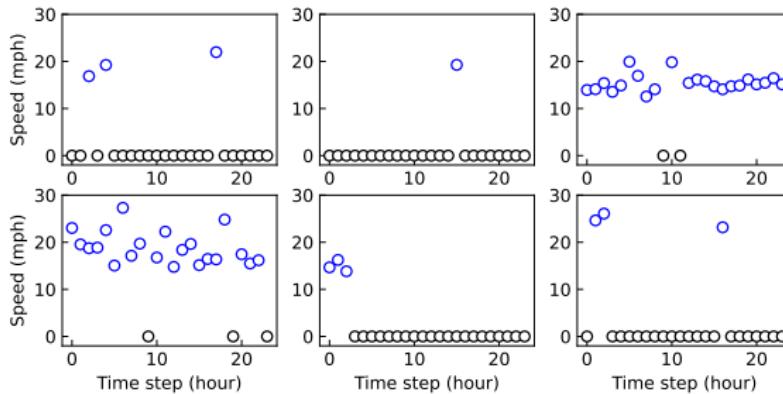


- **Seattle** movement speed data (2019)
  - **63,490** road segments & 8,760 time steps (hours)
  - Whole missing rate: **84.95%**



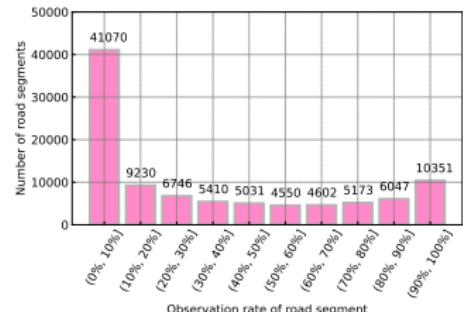
# Uber Movement Data

- [Examples] Movement speed of 6 road segments on Jan. 1, 2019 in NYC.



- [Stats] Missing rate w.r.t. road segments in NYC movement data:

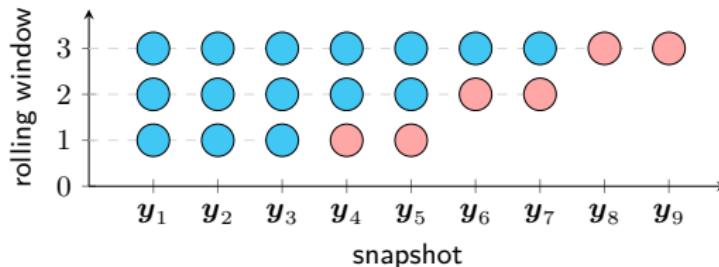
- $\approx 42\%$  road segments are with more than 90% missing values.
- $\approx 51\%$  road segments are with more than 80% missing values.
- $\approx 11\%$  road segments are with less than 10% missing values.



# Experiments

## Experiment setup

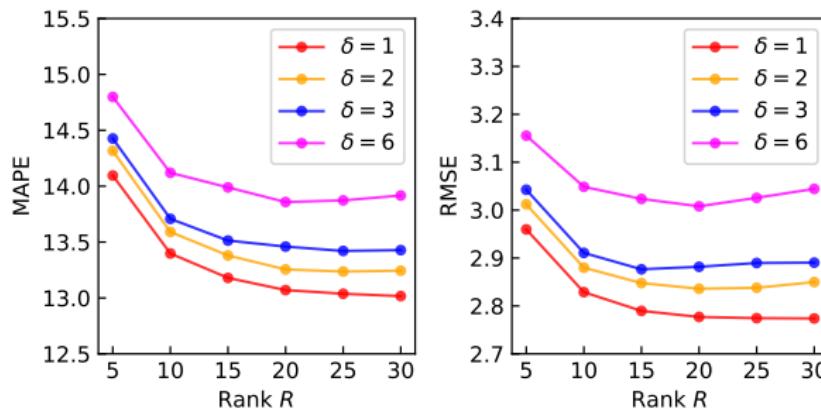
- NYC movement speed dataset:
  - Ten-week data of size  $98210 \times 1680$
  - Contain 66.56% missing values
- Rolling forecasting setup:
  - Training set: 8-week data
  - Validation set: 1-week data
  - Test set: 1-week data
  - Time horizon:  $\delta = 1, 2, 3, 6$
- Rolling forecasting illustration ( $\delta = 2$ ):



# Experiments

## Rank selection

- A larger rank essentially provides higher accuracy but the increase becomes marginal when  $R > 15$ .
- We choose  $R = 10$  for a good balance between performance and computational cost.



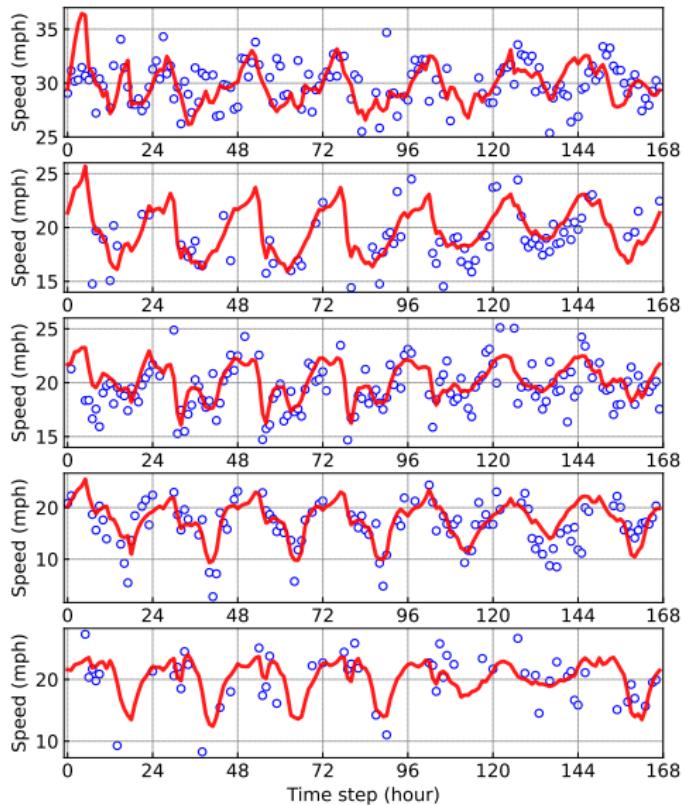
# Experiments

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## Findings:

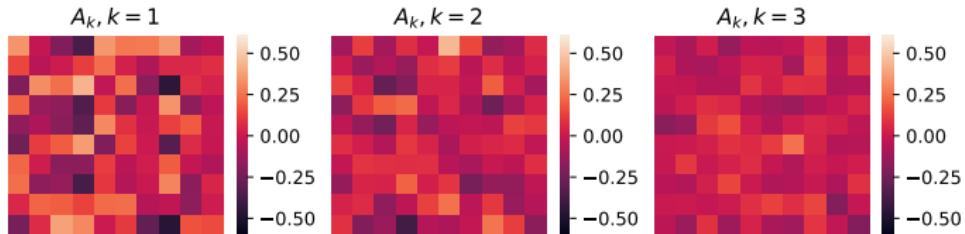
- NoTMF outperforms other models.
- Seasonal differencing in NoTMF is important.

$\delta$	$d$	NoTMF ( $m = 24$ )	NoTMF ( $m = 168$ )	NoTMF-twice ( $m = 168$ )	TMF	TRMF	BTMF
1	1	13.63/2.88	13.53/2.86	<b>13.45/2.85</b>	13.74/2.90	14.50/3.12	14.94/3.13
	2	<b>13.47/2.84</b>	<b>13.41/2.84</b>	13.42/2.84	13.53/2.85	14.14/3.05	15.70/3.41
	3	13.46/2.84	<b>13.39/2.83</b>	13.43/2.84	<b>13.47/2.83</b>	13.87/2.96	15.80/3.34
	6	13.41/2.83	<b>13.39/2.83</b>	13.41/2.83	<b>13.40/2.83</b>	14.00/2.98	15.45/3.27
2	1	13.91/2.96	13.76/2.94	<b>13.70/2.92</b>	14.24/3.00	15.85/3.43	15.33/3.21
	2	13.77/2.92	<b>13.63/2.89</b>	13.72/2.92	13.87/2.91	15.04/3.31	15.87/3.32
	3	13.72/2.91	<b>13.61/2.89</b>	13.73/2.92	<b>13.81/2.89</b>	15.25/3.36	15.69/3.33
	6	13.59/2.87	<b>13.57/2.88</b>	13.68/2.91	<b>13.63/2.86</b>	14.92/3.24	15.91/3.39
3	1	14.30/3.05	14.06/3.02	<b>14.02/3.00</b>	14.81/3.12	17.52/3.83	15.86/3.32
	2	14.01/2.98	<b>13.84/2.94</b>	13.96/2.98	14.26/2.98	17.32/4.00	16.30/3.40
	3	13.95/2.97	<b>13.79/2.93</b>	13.98/2.98	14.04/2.94	16.91/3.71	16.56/3.49
	6	13.78/2.92	<b>13.73/2.92</b>	13.91/2.96	<b>13.94/2.92</b>	16.72/3.65	15.49/3.27
6	1	<b>14.61/3.11</b>	14.67/3.20	14.98/3.32	15.41/3.21	21.20/4.70	15.99/3.32
	2	<b>14.30/3.03</b>	14.33/3.09	14.90/3.28	14.85/3.07	20.87/5.01	16.04/3.33
	3	<b>14.26/3.03</b>	14.28/3.09	14.86/3.26	<b>14.57/3.01</b>	20.08/4.65	15.67/3.28
	6	<b>14.06/2.97</b>	14.16/3.06	14.80/3.23	14.47/3.00	20.40/4.35	16.38/3.50

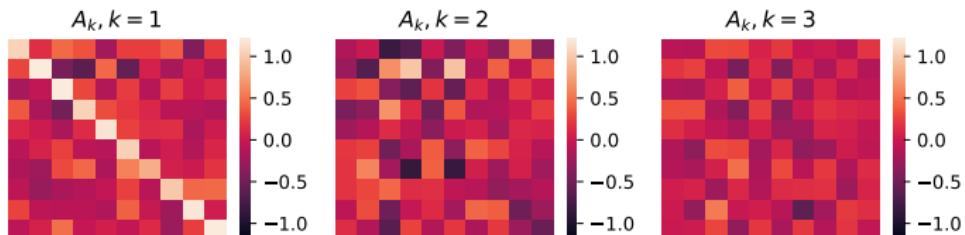


## Observing $A$

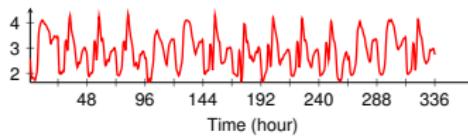
- NoTMF: showing weak correlations after differencing.



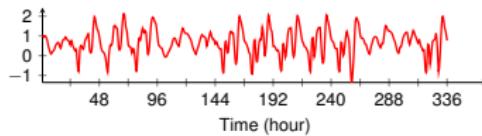
- TMF: showing strong autocorrelations in  $A_1$  (see diagonal entries).



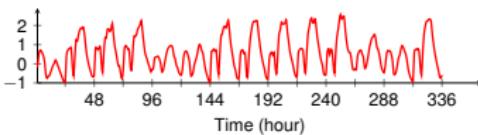
Temporal factor #1



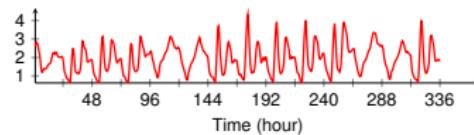
Temporal factor #2



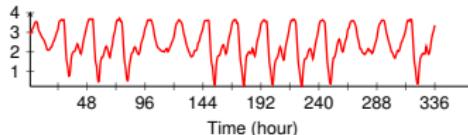
Temporal factor #3



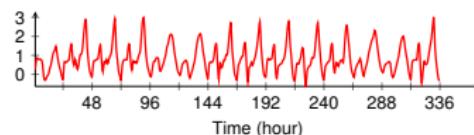
Temporal factor #4



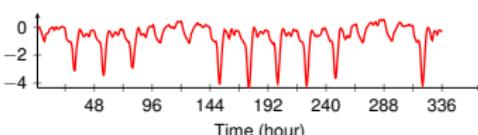
Temporal factor #5



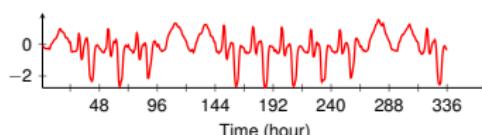
Temporal factor #6



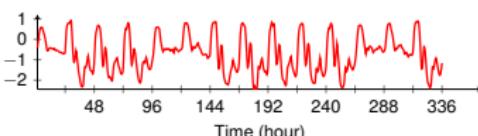
Temporal factor #7



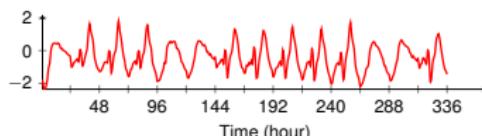
Temporal factor #8



Temporal factor #9



Temporal factor #10



# Concluding Remarks

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- Nonstationarity issue is important but mostly ignored.
  - e.g. the importance of stationarity in traffic forecasting (Rodrigues'22).
- Proper differencing operations are needed for addressing nonstationarity in real-world time series.

X. Chen, C. Zhang, X.L. Zhao, N. Saunier, L. Sun (2022). Nonstationary temporal matrix factorization for multivariate time series forecasting. arXiv preprint arXiv:2203.10651.

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## A short list:

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# Thanks for your attention!

## Any Questions?

### About me:

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