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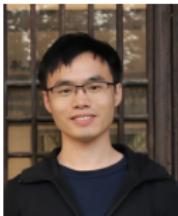
Matrix and Tensor Models for Spatiotemporal Traffic Data Imputation and Forecasting

Ph.D. Defense

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Outline

- **Background**
- **Literature Review**
 - Tensor Factorization
 - Tensor Factorization (TF)
- **Nonstationary Temporal Matrix Factorization**
- **Low-Rank Autoregressive Tensor Completion**
- **Laplacian Convolutional Representation**
 - Motivation
 - Reformulate Laplacian Regularization
 - Traffic Time Series Imputation
- **Hankel Tensor Factorization**
 - Motivation
 - Hankel Structure
 - Hankel Structure
- **Experiments**
- **Conclusion**

Our studies: (Pattern discovery, traffic data imputation/forecasting)

- ❶ X. Chen, C. Zhang, X. Chen, N. Saunier, L. Sun (2023). Discovering dynamic patterns from spatiotemporal data with time-varying low-rank autoregression. *IEEE Transactions on Knowledge and Data Engineering*. Early access.
- ❷ X. Chen, Z. Cheng, N. Saunier, L. Sun (2022). Laplacian convolutional representation for traffic time series imputation. *arXiv preprint arXiv:2212.01529*.
- ❸ X. Chen, L. Sun (2022). Bayesian temporal factorization for multidimensional time series prediction. *IEEE Transactions on Pattern Analysis and Machine Intelligence*. 44 (9): 4659-4673.

GitHub repository:

- **transdim**: Machine learning for spatiotemporal traffic data imputation and forecasting. (1,000 stars & 270 forks on GitHub)
<https://github.com/xinychen/transdim>

Problem Formulation

Imputation
Forecasting

Background
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Literature Review
○○

NoTMF
○

LATC
○

LCR
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HTF
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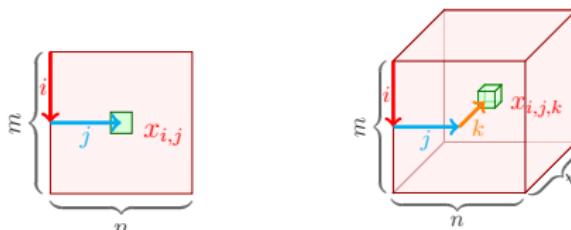
Experiments

Conclusion
○○

Whole Picture

Tensors

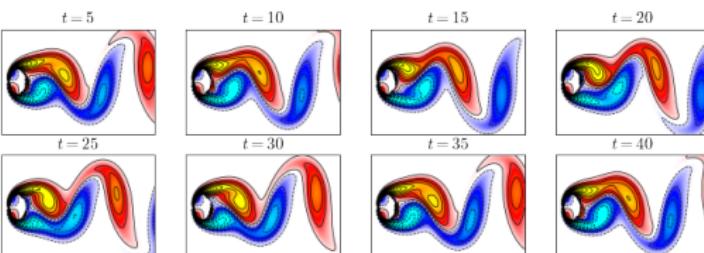
- What is tensor? $\mathbf{X} \in \mathbb{R}^{m \times n}$ vs. $\mathcal{X} \in \mathbb{R}^{m \times n \times t}$



- Tensors are everywhere!



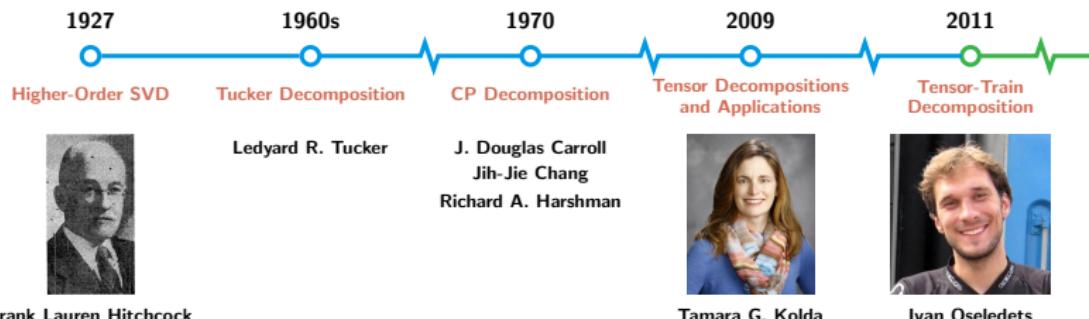
Color image with
RGB channels



Dynamical system (fluid flow)

Tensor Factorization

- Revisit tensor factorization (TF)

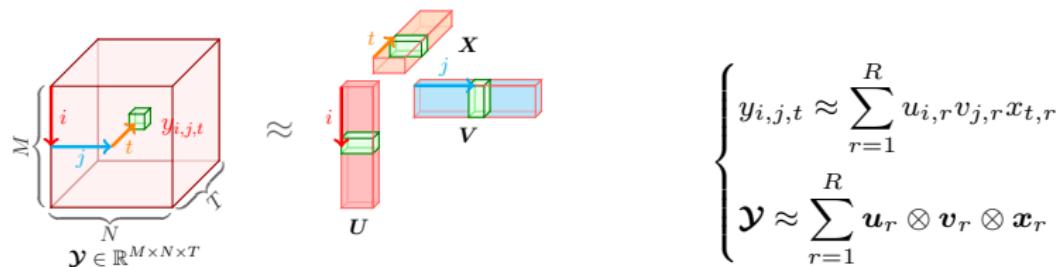


Frank Lauren Hitchcock

Tamara G. Kolda

Ivan Oseledets

- **CP tensor factorization:** Factorize \mathcal{Y} into the combination of three rank- R factor matrices (i.e., low-dimensional latent factors).



Background
oo

Literature Review
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NoTMF
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LATC
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LCR
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HTF
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Experiments

Conclusion
oo

TMF

Background
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Literature Review
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LCR
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Experiments

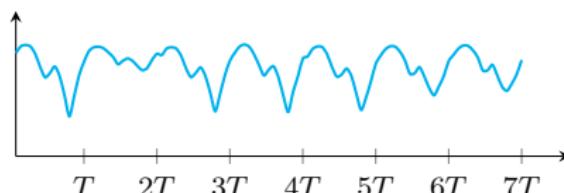
Conclusion
oo

LATC

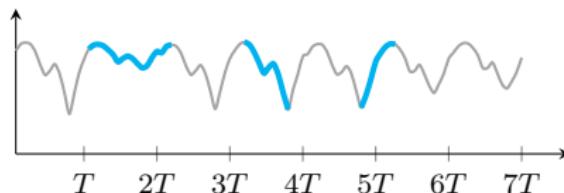
Laplacian Convolutional Representation

Motivation: Time series imputation

- Global trends (e.g., long-term quasi-seasonality & daily/weekly rhythm):



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



- [Question] How to characterize both global and local trends in sparse time series data?

Laplacian Convolutional Representation

[Local trend modeling] Reformulate temporal regularization with circular convolution.

- Intuition of (circulant) Laplacian matrix.

Undirected and circulant graph

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

(Circulant) Laplacian matrix

- Define Laplacian kernel:

$$\boldsymbol{\ell} \triangleq (2, -1, 0, 0, -1)^\top$$

↓

$$\boldsymbol{\ell} \triangleq (\underbrace{2\tau}_{\text{degree}}, \underbrace{-1, \dots, -1}_\tau, 0, \dots, 0, \underbrace{-1, \dots, -1}_\tau)^\top \in \mathbb{R}^T$$

for any time series $\mathbf{x} = (x_1, \dots, x_T)^\top \in \mathbb{R}^T$.

- (Laplacian) Temporal regularization:

$$\mathcal{R}_\tau(\mathbf{x}) = \frac{1}{2} \|\mathbf{L}\mathbf{x}\|_2^2 = \frac{1}{2} \|\boldsymbol{\ell} * \mathbf{x}\|_2^2$$

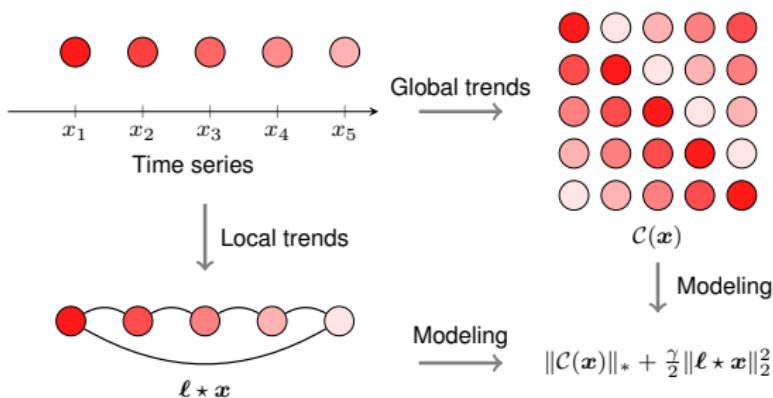
Laplacian Convolutional Representation

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 and local trends** in time series, respectively, i.e.,

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

where $\mathcal{C} : \mathbb{R}^T \rightarrow \mathbb{R}^{T \times T}$ denotes the circulant operator. $\|\cdot\|_*$ denotes the nuclear norm of matrix, namely, the sum of singular values.



Laplacian Convolutional Representation

- Augmented Lagrangian function:

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

where $\mathbf{w} \in \mathbb{R}^T$ is the Lagrange multiplier, and $\langle \cdot, \cdot \rangle$ denotes the inner product.

- The ADMM scheme:

$$\begin{cases} \mathbf{x} := \arg \min_{\mathbf{x}} \mathcal{L}(\mathbf{x}, \mathbf{z}, \mathbf{w}) & \text{(Nuclear norm minimization)} \\ \mathbf{z} := \arg \min_{\mathbf{z}} \mathcal{L}(\mathbf{x}, \mathbf{z}, \mathbf{w}) & \text{(Closed-form solution)} \\ = \frac{1}{\lambda + \eta} \mathcal{P}_\Omega(\lambda \mathbf{x} + \mathbf{w} + \eta \mathbf{y}) + \frac{1}{\lambda} \mathcal{P}_\Omega^\perp(\lambda \mathbf{x} + \mathbf{w}) \\ \mathbf{w} := \mathbf{w} + \lambda(\mathbf{x} - \mathbf{z}) & \text{(Standard update)} \end{cases}$$

- Optimize \mathbf{x} ?

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

Nuclear norm minimization \Rightarrow **ℓ_1 -norm minimization with FFT** (in $\mathcal{O}(T \log T)$ time).

Laplacian Convolutional Representation

- Optimize \mathbf{x} via FFT (in $\mathcal{O}(T \log T)$ time):

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

where we introduce $\{\hat{\ell}, \hat{\mathbf{x}}, \hat{\mathbf{z}}, \hat{\mathbf{w}}\} \triangleq \mathcal{F}\{\ell, \mathbf{x}, \mathbf{z}, \mathbf{w}\}$ (i.e., FFT).

ℓ_1 -norm Minimization in Complex Space (Liu & Zhang'23)

For any optimization problem in the form of ℓ_1 -norm minimization in complex space:

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

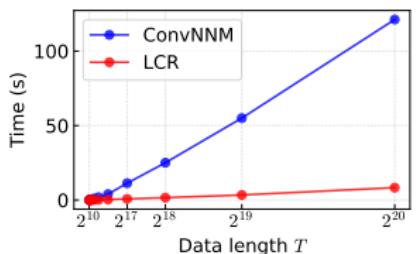
with complex-valued vectors $\hat{\mathbf{x}}, \hat{\mathbf{h}} \in \mathbb{C}^T$ and weight parameter ω , element-wise, the solution is given by

$$\hat{x}_t := \frac{\hat{h}_t}{|\hat{h}_t|} \cdot \max\{0, |\hat{h}_t| - 1/\omega\}, t = 1, \dots, T.$$

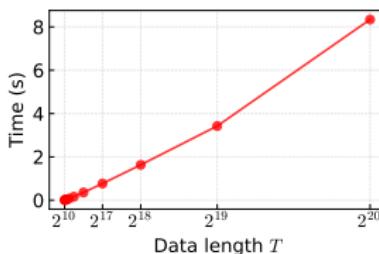
Laplacian Convolutional Representation

[Empirical time complexity] On $\mathbf{y} \in \mathbb{R}^T$ with $T \in \{2^{10}, 2^{11}, \dots, 2^{20}\}$

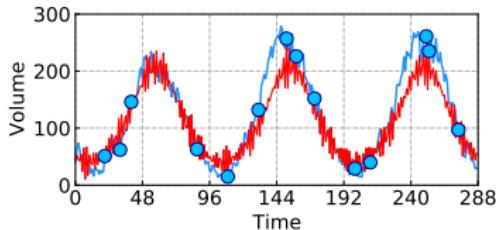
- Ours: **LCR**
 - An FFT implementation in $\mathcal{O}(T \log T)$
 - The logarithmic factor $\log T$ makes the FFT highly efficient
- Baseline: **ConvNNM** (Convolution nuclear norm minimization, Liu & Zhang'23)
 - Convolution matrix $\mathcal{C}_{\tilde{\tau}}(\mathbf{y}) \in \mathbb{R}^{T \times \tilde{\tau}}$ with kernel size $\tilde{\tau} \in \mathbb{N}^+$
 - Singular value thresholding in $\mathcal{O}(\tilde{\tau}^2 T)$



ConvNNM vs. LCR



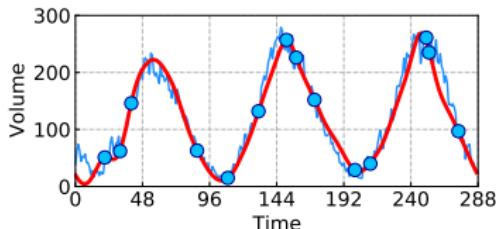
LCR



CircNNM:

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

↓ Plus temporal regularization (TR)

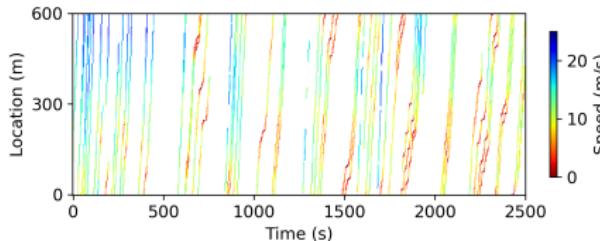


LCR:

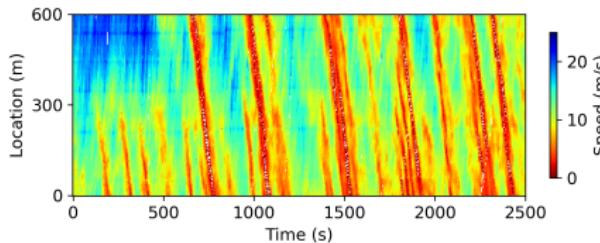
$$\begin{aligned} & \min_{\boldsymbol{x}} \|\mathcal{C}(\boldsymbol{x})\|_* + \frac{\gamma}{2} \|\boldsymbol{\ell} * \boldsymbol{x}\|_2^2 \\ \text{s. t. } & \|\mathcal{P}_\Omega(\boldsymbol{x} - \boldsymbol{y})\|_2 \leq \epsilon \end{aligned}$$

Motivation: Spatiotemporal data reconstruction

- Speed field reconstruction problem in vehicular traffic flow.



200-by-500 matrix
(NGSIM) \Downarrow Reconstruct speed field from
5% sparse trajectories?

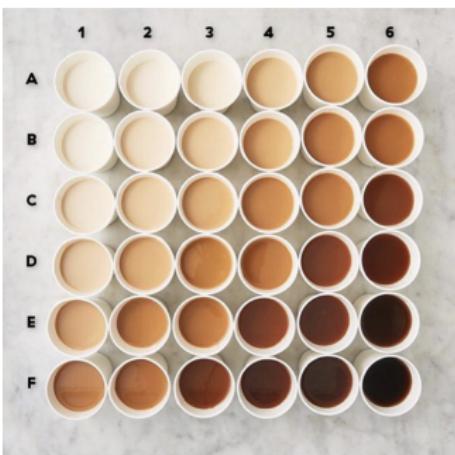


- How to learn from sparse spatiotemporal data?
- How to characterize spatial/temporal dependencies?

Hankel Tensor Factorization

- Hankel matrix
 - Given $\mathbf{x} = (1, 2, 3, 4, 5)^\top$ and window length $\tau = 2$, we have

$$\mathcal{H}_\tau(\mathbf{x}) = \begin{bmatrix} 1 & 2 \\ 2 & 3 \\ 3 & 4 \\ 4 & 5 \end{bmatrix} \in \mathbb{R}^{4 \times 2}$$



Hankel matrix (Source: Twitter)

Hankel Tensor Factorization

- Hankel matrix

- On time series $\mathbf{y} = (y_1, y_2, \dots, y_5)^\top$ with $\tau = 2$:

$$\mathcal{H}_\tau(\mathbf{y}) = \begin{bmatrix} y_1 & y_2 \\ y_2 & y_3 \\ y_3 & y_4 \\ y_4 & y_5 \end{bmatrix} \approx \begin{bmatrix} v_1 \\ v_2 \\ v_3 \\ v_4 \end{bmatrix} \otimes \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}$$

$$\implies \hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \hat{y}_4 \\ \hat{y}_5 \end{bmatrix} = \mathcal{H}_\tau^{-1} \left(\begin{bmatrix} v_1 x_1 & v_1 x_2 \\ v_2 x_1 & v_2 x_2 \\ v_3 x_1 & v_3 x_2 \\ v_4 x_1 & v_4 x_2 \end{bmatrix} \right) = \begin{bmatrix} v_1 x_1 \\ (v_1 x_2 + v_2 x_1)/2 \\ (v_2 x_2 + v_3 x_1)/2 \\ (v_3 x_2 + v_4 x_1)/2 \\ v_4 x_2 \end{bmatrix}$$

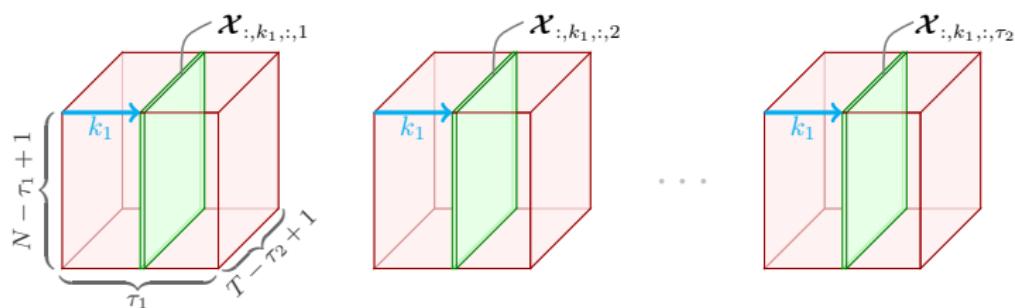
- Automatic temporal modeling.

Hankel Tensor Factorization

- Hankel tensor: Given any matrix $\mathbf{X} \in \mathbb{R}^{N \times T}$, we have

$$\mathcal{X} \triangleq \mathcal{H}_{\tau_1, \tau_2}(\mathbf{X})$$

- Window lengths: $\tau_1, \tau_2 \in \mathbb{N}^+$;
- Tensor size: $(N - \tau_1 + 1) \times \tau_1 \times (T - \tau_2 + 1) \times \tau_2$;



(Figure) 4th order Hankel tensor: A sequence of third-order tensors.

- Slice: $\mathcal{X}_{:,k_1,:,:,\tau_2}, \forall k_1, k_2$;
- Slice size: $(N - \tau_1 + 1) \times (T - \tau_2 + 1)$.

Hankel Tensor Factorization

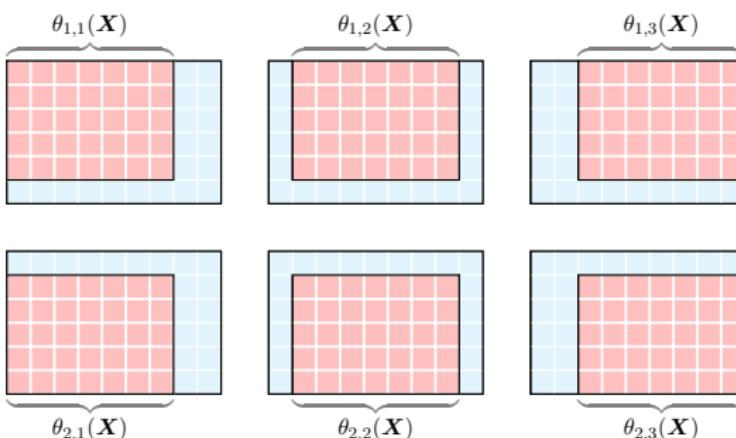
Hankel indexing:

- Sampling function for the Hankelization:

$$\theta_{k_1, k_2}(\mathbf{X}) \triangleq [\mathcal{H}_{\tau_1, \tau_2}(\mathbf{X})]_{:, k_1, :, k_2},$$

referring to the tensor slice with $k_1 \in \{1, \dots, \tau_1\}$, $k_2 \in \{1, \dots, \tau_2\}$.

- [Importance]** Developing memory-efficient algorithms.



- Tensor slices $\theta_{k_1, k_2}(\mathbf{X})$ vs. data matrix \mathbf{X}

Hankel Tensor Factorization

Our model:

- Convolutional tensor decomposition (circular convolution \star_{row}):

$$\theta_{k_1, k_2}(\mathbf{Y}) \approx (\mathbf{Q} \star_{\text{row}} \mathbf{s}_{k_1}^{\top})(\mathbf{U} \star_{\text{row}} \mathbf{v}_{k_2}^{\top})^{\top}$$

Baselines:

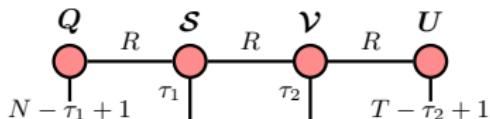
- CP tensor decomposition (Khatri-Rao product \odot):

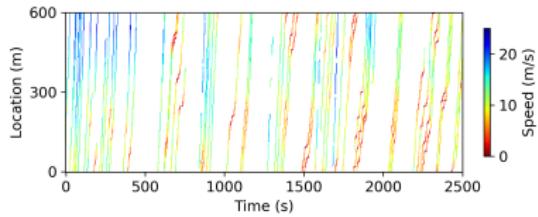
$$\theta_{k_1, k_2}(\mathbf{Y}) \approx (\mathbf{Q} \odot \mathbf{s}_{k_1}^{\top})(\mathbf{U} \odot \mathbf{v}_{k_2}^{\top})^{\top}$$

- Tensor-train decomposition:

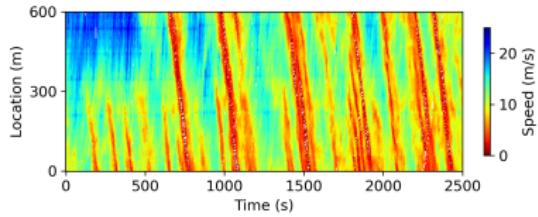
$$\theta_{k_1, k_2}(\mathbf{Y}) \approx (\mathbf{Q} \mathbf{S}_{k_1})(\mathbf{U} \mathbf{V}_{k_2})^{\top}$$

- $\{\mathbf{S}_{k_1}, \mathbf{V}_{k_2}\}$ are **circulant matrices** \Rightarrow convolutional decomposition
- $\{\mathbf{S}_{k_1}, \mathbf{V}_{k_2}\}$ are **diagonal matrices** \Rightarrow CP decomposition

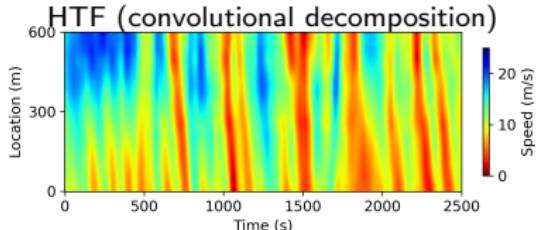




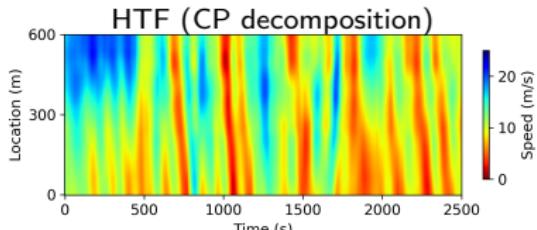
Sparse speed field



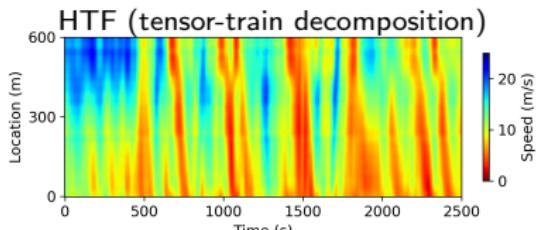
Ground truth speed field



MAPE = 51.92%



MAPE = 53.93%



MAPE = 56.48%

Conclusion

Time-Varying Autoregression:

- (Highlight) Interpretable model with tensor factorization.
 - ✓ Parameter compression ✓ Pattern discovery

Laplacian Convolutional Representation:

- (Solution) Time series trend modeling in the low-rank framework?
 - Global time series trend modeling (low-rank model):

$$\begin{aligned} \min_{\mathbf{x}} & \quad \|\mathcal{C}(\mathbf{x})\|_* \\ \text{s. t. } & \quad \|\mathcal{P}_\Omega(\mathbf{x} - \mathbf{y})\|_2 \leq \epsilon \end{aligned}$$

- Local time series trend modeling (temporal regularization):

$$\mathcal{R}_\tau(\mathbf{x}) = \frac{1}{2} \|\boldsymbol{\ell} * \mathbf{x}\|_2^2$$

- (Highlight) A unified framework with the **FFT** implementation.

Hankel Tensor Factorization:

- (Highlight) Memory-efficient **Hankel indexing & convolutional parameterization**.



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Thank you for your attention!

Any Questions?

About me:

- 🏠 Homepage: <https://xinychen.github.io>
- /github/ GitHub: <https://github.com/xinychen>
- ✉️ How to reach me: chenxy346@gmail.com

Appendix

HTF (convolutional decomposition)

- Optimization problem:

$$\begin{aligned} \min_{\mathbf{Q}, \mathbf{S}, \mathbf{U}, \mathbf{V}} \quad & \frac{1}{2} \sum_{k_1, k_2} \left\| \mathcal{P}_{\Omega_{k_1, k_2}} (\theta_{k_1, k_2}(\mathbf{Y}) - (\mathbf{Q} \star_{\text{row}} \mathbf{s}_{k_1})(\mathbf{U} \star_{\text{row}} \mathbf{v}_{k_2})^\top) \right\|_F^2 \\ & + \frac{\rho}{2} (\|\mathbf{Q}\|_F^2 + \|\mathbf{S}\|_F^2 + \|\mathbf{U}\|_F^2 + \|\mathbf{V}\|_F^2) \end{aligned}$$

- Alternating minimization:

$$\left\{ \begin{array}{l} \mathbf{Q} := \{\mathbf{Q} \mid \frac{\partial f}{\partial \mathbf{Q}} = \mathbf{0}\} \\ \mathbf{s}_{k_1} := \{\mathbf{s}_{k_1} \mid \frac{\partial f}{\partial \mathbf{s}_{k_1}} = \mathbf{0}\}, \quad k_1 \in \{1, 2, \dots, \tau_1\} \\ \mathbf{U} := \{\mathbf{U} \mid \frac{\partial f}{\partial \mathbf{U}} = \mathbf{0}\} \\ \mathbf{v}_{k_2} := \{\mathbf{v}_{k_2} \mid \frac{\partial f}{\partial \mathbf{v}_{k_2}} = \mathbf{0}\}, \quad k_2 \in \{1, 2, \dots, \tau_2\} \end{array} \right.$$