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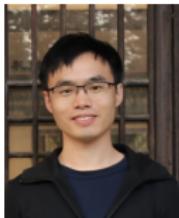
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# Low-Rank Matrix and Tensor Factorization for Speed Field Reconstruction

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## Source

- ① **Slides:** [https://xinychen.github.io/slides/MF\\_TF\\_SFR.pdf](https://xinychen.github.io/slides/MF_TF_SFR.pdf)
- ② **Jupyter Notebook:** [https://github.com/xinychen/transdim/blob/master/toy-examples/MF\\_TF\\_SFR.ipynb](https://github.com/xinychen/transdim/blob/master/toy-examples/MF_TF_SFR.ipynb)

# Outline

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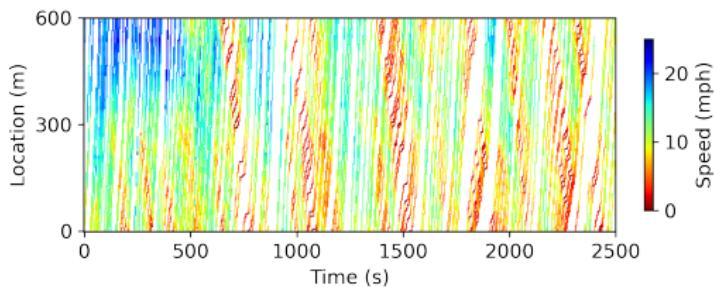
- **Motivation**
- **Matrix Factorization**
  - Optimization Problem
  - GD vs. SGD vs. ALS
- **Smoothing Matrix Factorization**
  - Spatial/Temporal Smoothing
  - Alternating Minimization
- **Tensor Factorization**
  - Basic Idea
  - CP Tensor Factorization
  - Hankel Tensor and Its Factorization
- **Discussion**
  - Which Model Is Better?

# Motivation

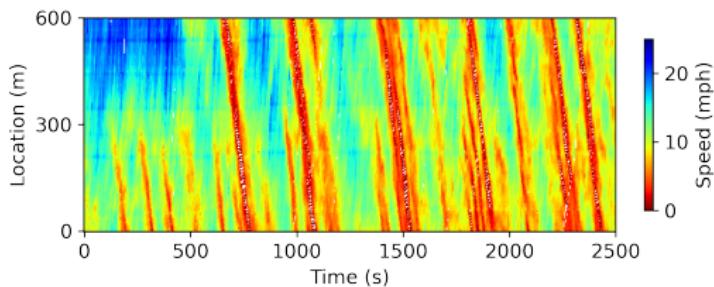
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# Motivation

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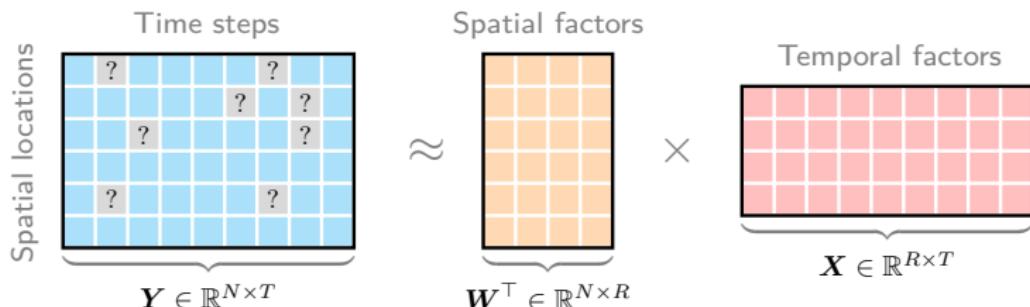
200-by-500 matrix  
(NGSIM)  $\Downarrow$  Reconstruct speed field  
from sparse trajectories?



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

# Matrix Factorization

- Spatiotemporal data can be reconstructed by low-dimensional latent factors!



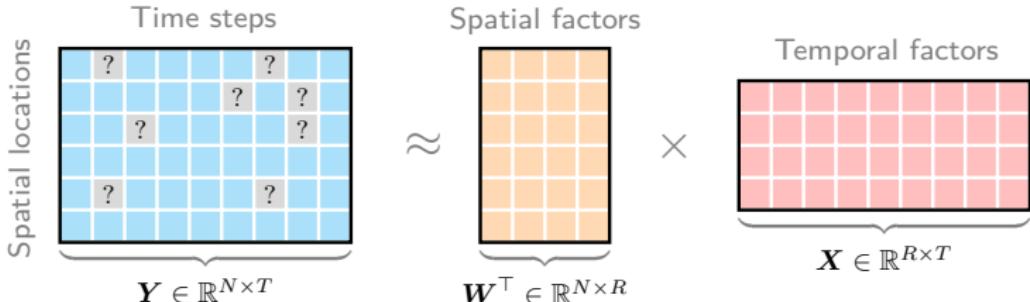
- MF optimization problem

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

with factor matrices  $\mathbf{W}$  and  $\mathbf{X}$ .

- Objective function  $f(\mathbf{W}, \mathbf{X})$  or  $f$ ;
- Rank  $R \in \mathbb{N}^+$  ( $R < \min\{N, T\}$ );
- Orthogonal projection  $\mathcal{P}_\Omega(\cdot)$ .

# Matrix Factorization



- MF optimization problem

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

- Orthogonal projection  $\mathcal{P}_\Omega : \mathbb{R}^{N \times T} \rightarrow \mathbb{R}^{N \times T}$ ?

- Simple example:  $\mathbf{Y} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$  with  $\Omega = \{(1, 1), (2, 2)\}$ , we have

$$\mathcal{P}_\Omega(\mathbf{Y}) = \begin{bmatrix} 1 & 0 \\ 0 & 4 \end{bmatrix} \quad \mathcal{P}_\Omega^\perp(\mathbf{Y}) = \begin{bmatrix} 0 & 2 \\ 3 & 0 \end{bmatrix} \quad (\text{On the complement})$$

- Role of regularization (with  $\rho$ ): avoid overfitting.

# Matrix Factorization

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- MF optimization problem

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

- Partial derivatives

$$\begin{cases} \frac{\partial f}{\partial \mathbf{W}} = -\mathbf{X} \mathcal{P}_\Omega^\top (\mathbf{Y} - \mathbf{W}^\top \mathbf{X}) + \rho \mathbf{W} \\ \frac{\partial f}{\partial \mathbf{X}} = -\mathbf{W} \mathcal{P}_\Omega (\mathbf{Y} - \mathbf{W}^\top \mathbf{X}) + \rho \mathbf{X} \end{cases}$$

- Gradient descent (**GD**) vs. Steepest gradient descent (**SGD**)

$$\begin{cases} \mathbf{W} := \mathbf{W} - \alpha \frac{\partial f}{\partial \mathbf{W}} \\ \mathbf{X} := \mathbf{X} - \alpha \frac{\partial f}{\partial \mathbf{X}} \end{cases} \quad \text{vs.} \quad \begin{cases} \alpha := \arg \min_\alpha f(\mathbf{W} - \alpha \frac{\partial f}{\partial \mathbf{W}}, \mathbf{X}) \\ \mathbf{W} := \mathbf{W} - \alpha \frac{\partial f}{\partial \mathbf{W}} \\ \beta := \arg \min_\beta f(\mathbf{W}, \mathbf{X} - \beta \frac{\partial f}{\partial \mathbf{X}}) \\ \mathbf{X} := \mathbf{X} - \beta \frac{\partial f}{\partial \mathbf{X}} \end{cases}$$

- Fixed step size  $\alpha$  (**GD**) vs. optimal step sizes  $\{\alpha, \beta\}$  (**SGD**)

# Matrix Factorization

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- MF optimization problem

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

- Partial derivatives

$$\begin{cases} \frac{\partial f}{\partial \mathbf{W}} = -\mathbf{X} \mathcal{P}_\Omega^\top (\mathbf{Y} - \mathbf{W}^\top \mathbf{X}) + \rho \mathbf{W} \\ \frac{\partial f}{\partial \mathbf{X}} = -\mathbf{W} \mathcal{P}_\Omega (\mathbf{Y} - \mathbf{W}^\top \mathbf{X}) + \rho \mathbf{X} \end{cases}$$

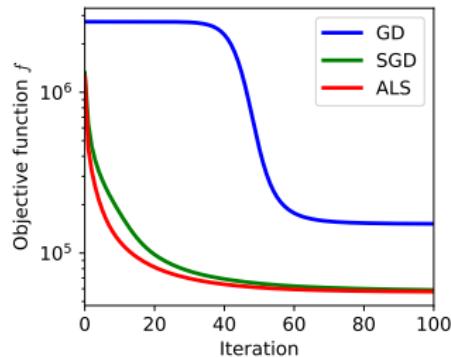
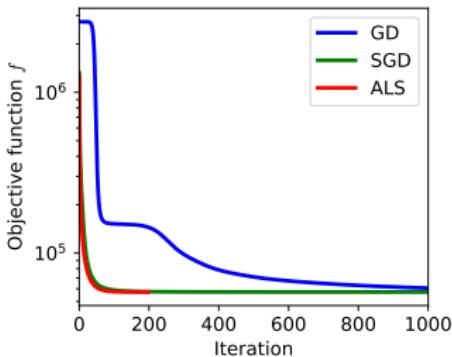
- Alternating least squares (**ALS**)

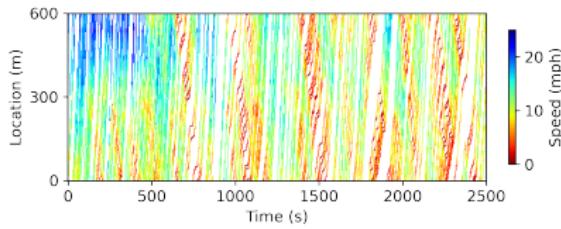
$$\begin{cases} \mathbf{w}_i := \left( \sum_{t:(i,t) \in \Omega} \mathbf{x}_t \mathbf{x}_t^\top + \rho \mathbf{I}_R \right)^{-1} \sum_{t:(i,t) \in \Omega} \mathbf{x}_t y_{i,t} \\ \mathbf{x}_t := \left( \sum_{i:(i,t) \in \Omega} \mathbf{w}_i \mathbf{w}_i^\top + \rho \mathbf{I}_R \right)^{-1} \sum_{i:(i,t) \in \Omega} \mathbf{w}_i y_{i,t} \end{cases}$$

- $\mathbf{w}_i \in \mathbb{R}^R$ ,  $i = 1, 2, \dots, N$  are the columns of  $\mathbf{W}$ ;
- $\mathbf{x}_t \in \mathbb{R}^R$ ,  $t = 1, 2, \dots, T$  are the columns of  $\mathbf{X}$ .

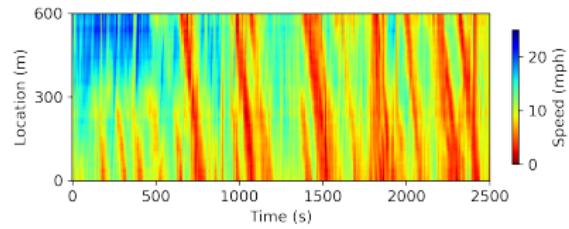
# Matrix Factorization

- Objective function  $f$  vs. iteration
  - Set rank  $R = 10$ , weight parameter  $\rho = 10$ ;
  - Set GD step size  $\alpha = 10^{-4}$ .

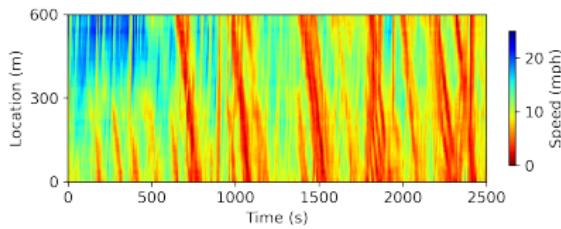




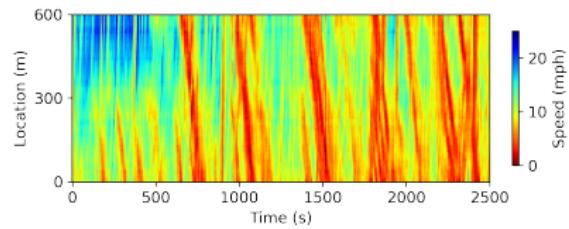
Sparse speed field



MF with GD



MF with SGD



MF with ALS

- Reconstruction errors

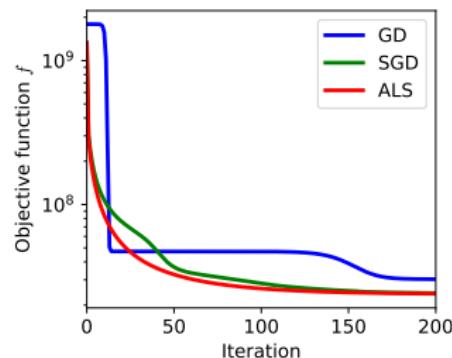
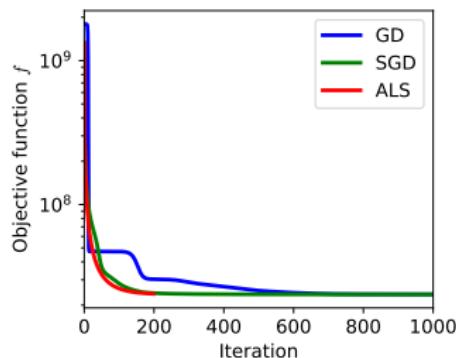
$$\text{MAPE} = \begin{cases} 50.66\% & (\text{GD}) \\ 45.13\% & (\text{SGD}) \\ 45.84\% & (\text{ALS}) \end{cases}$$

$$\text{RMSE} = \begin{cases} 2.33 & (\text{GD}) \\ 2.79 & (\text{SGD}) \quad (\text{mph}) \\ 2.80 & (\text{ALS}) \end{cases}$$

# Matrix Factorization

**Seattle freeway speed dataset** (randomly generate 60% missing values)

- Objective function  $f$  vs. iteration
  - Rank  $R = 10$ , weight parameter  $\rho = 10^2$ ;
  - GD step size  $\alpha = 2 \times 10^{-5}$ .



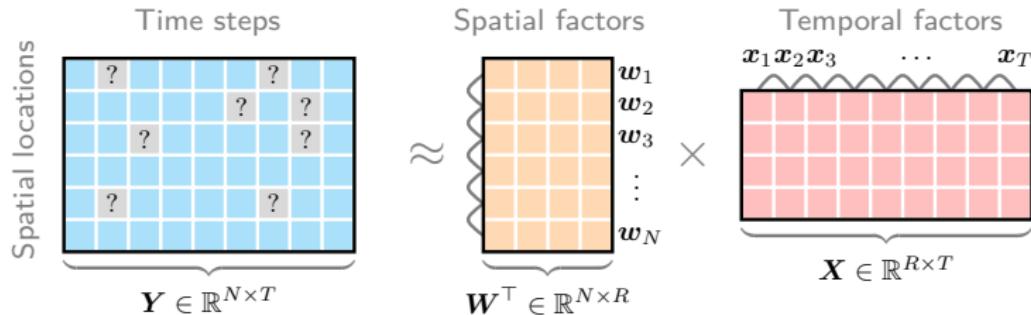
- Reconstruction errors

$$\text{MAPE} = \begin{cases} 9.14\% & (\text{GD}) \\ 9.12\% & (\text{SGD}) \\ 9.13\% & (\text{ALS}) \end{cases}$$

$$\text{RMSE} = \begin{cases} 5.24 & (\text{GD}) \\ 5.24 & (\text{SGD}) \quad (\text{mph}) \\ 5.24 & (\text{ALS}) \end{cases}$$

# Smoothing Matrix Factorization

- Spatial/temporal local dependencies are also important!



- Formulate spatial/temporal dependencies

$$\mathbf{W}\Psi_1^\top = \begin{bmatrix} & | & & | \\ \mathbf{w}_2 - \mathbf{w}_1 & \cdots & \mathbf{w}_N - \mathbf{w}_{N-1} & \\ & | & & | \end{bmatrix}$$
$$\mathbf{X}\Psi_2^\top = \begin{bmatrix} & | & & | \\ \mathbf{x}_2 - \mathbf{x}_1 & \cdots & \mathbf{x}_T - \mathbf{x}_{T-1} & \\ & | & & | \end{bmatrix}$$

# Smoothing Matrix Factorization

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- Formulate spatial/temporal dependencies

$$\Psi = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ 0 & 0 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix} \implies \begin{cases} \mathbf{W}\Psi_1^\top & \text{with } \Psi_1 \in \mathbb{R}^{(N-1) \times N} \\ \mathbf{X}\Psi_2^\top & \text{with } \Psi_2 \in \mathbb{R}^{(T-1) \times T} \end{cases}$$

- SMF optimization problem

$$\begin{aligned} \min_{\mathbf{W}, \mathbf{X}} \quad & \frac{1}{2} \left\| \mathcal{P}_\Omega(\mathbf{Y} - \mathbf{W}^\top \mathbf{X}) \right\|_F^2 + \frac{\rho}{2} (\|\mathbf{W}\|_F^2 + \|\mathbf{X}\|_F^2) \\ & + \frac{\lambda}{2} (\|\mathbf{W}\Psi_1^\top\|_F^2 + \|\mathbf{X}\Psi_2^\top\|_F^2) \end{aligned}$$

- **Alternating minimization**

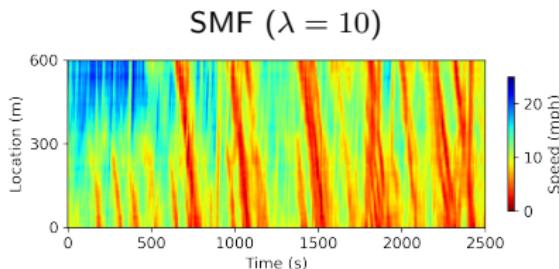
$$\mathbf{W} := \{ \mathbf{W} \mid \frac{\partial f}{\partial \mathbf{W}} = \mathbf{0} \} \quad \mathbf{X} := \{ \mathbf{X} \mid \frac{\partial f}{\partial \mathbf{X}} = \mathbf{0} \}$$

- Solving each matrix equation by the **conjugate gradient** method.

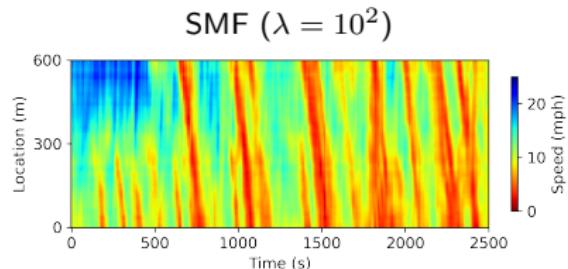
# Smoothing Matrix Factorization

- Speed field reconstruction
  - Rank  $R = 10$ , weight parameter  $\rho = 10$ .
  - Recall that the reconstruction errors of MF:

$$\text{MAPE} = \begin{cases} 50.66\% & (\text{GD}) \\ 45.13\% & (\text{SGD}) \\ 45.84\% & (\text{ALS}) \end{cases} \quad \text{RMSE} = \begin{cases} 2.33 & (\text{GD}) \\ 2.79 & (\text{SGD}) \quad (\text{mph}) \\ 2.80 & (\text{ALS}) \end{cases}$$



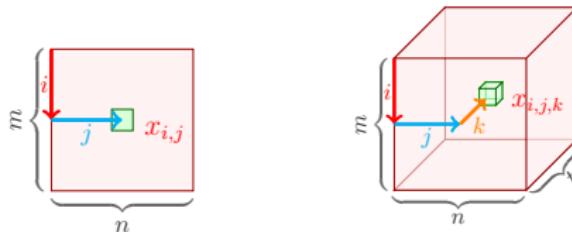
MAPE = 44.06%, RMSE = 2.16mph



MAPE = 48.00%, RMSE = 1.60mph

# Tensor Factorization

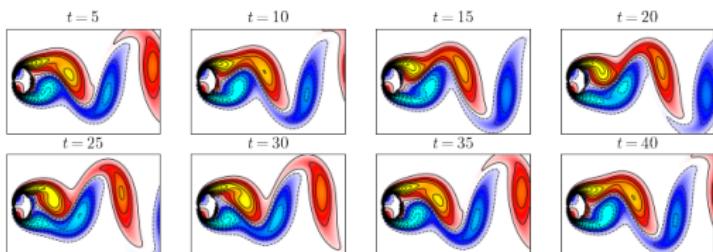
- What is tensor?  $X \in \mathbb{R}^{m \times n}$  vs.  $\mathcal{X} \in \mathbb{R}^{m \times n \times t}$



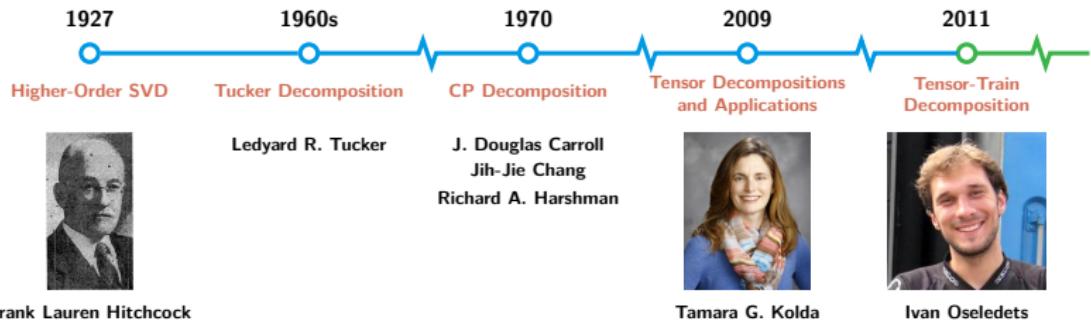
- Real-world tensors



Color image with  
RGB channels

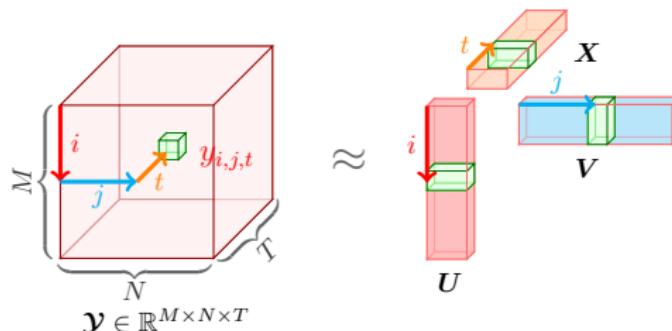


Dynamical system (fluid flow)



# CP Tensor Factorization

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



- Understanding CP factorization<sup>1</sup>:

$$\left\{ \begin{array}{l} y_{i,j,t} \approx \sum_{r=1}^R u_{i,r} v_{j,r} x_{t,r} \quad (\text{sum of latent factors}) \\ \mathcal{Y} \approx \sum_{r=1}^R \mathbf{u}_r \otimes \mathbf{v}_r \otimes \mathbf{x}_r \quad (\text{sum of rank-one tensors}) \end{array} \right.$$

<sup>1</sup>The symbol  $\otimes$  denotes the outer product.

# Hankel Tensor and Its Factorization

- Hankel matrix

- Given  $\mathbf{y} = (1, 2, 3, 4, 5, 6)^\top$  and window length  $\tau = 3$ , we have

$$\mathcal{H}_\tau(\mathbf{y}) = \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 4 \\ 3 & 4 & 5 \\ 4 & 5 & 6 \end{bmatrix} \in \mathbb{R}^{4 \times 3}$$

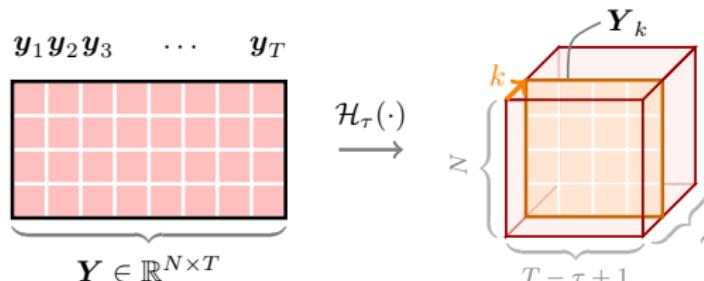
- On time series?

- (Hankelization) Hankel tensor  $\mathcal{H}_\tau(\mathbf{Y})$

- Tensor size:  $N \times (T - \tau + 1) \times \tau$ ;

- Slices:  $\mathbf{Y}_k = \begin{bmatrix} | & | & | & | \\ \mathbf{y}_k & \mathbf{y}_{k+1} & \cdots & \mathbf{y}_{T-\tau+k} \\ | & | & | & | \end{bmatrix}, k = 1, 2, \dots, \tau$ ;

- Slice size:  $N \times (T - \tau + 1)$ .



# Hankel Tensor and Its Factorization

- HTF optimization problem

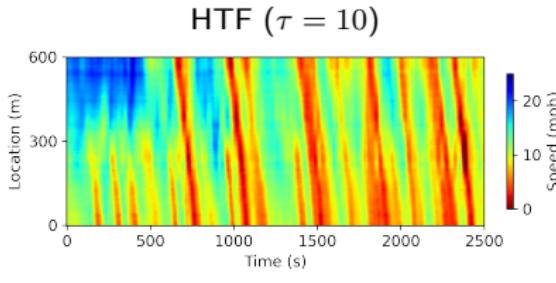
$$\begin{aligned} \min_{\mathbf{U}, \mathbf{V}, \mathbf{X}} \quad & \frac{1}{2} \left\| \mathcal{P}_{\Omega} \left( \mathcal{H}_{\tau}(\mathbf{Y}) - \sum_{r=1}^R \mathbf{u}_r \otimes \mathbf{v}_r \otimes \mathbf{x}_r \right) \right\|_F^2 \\ & + \frac{\rho}{2} (\|\mathbf{U}\|_F^2 + \|\mathbf{V}\|_F^2 + \|\mathbf{X}\|_F^2) \end{aligned}$$

- HTF's advantage/disadvantage over MF:

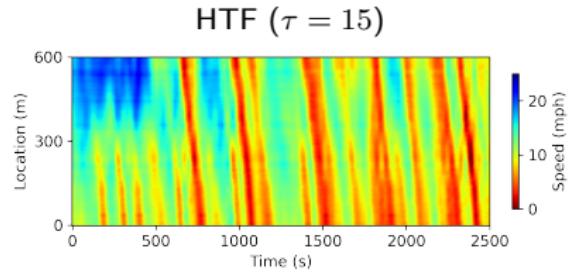
- ✓ Automatic temporal modeling
- ✗ High memory consumption

- Speed field reconstruction

- Set rank  $R = 10$ , weight parameter  $\rho = 10$ ;
- Recall that SMF: MAPE = 48.00% & RMSE = 1.60mph.

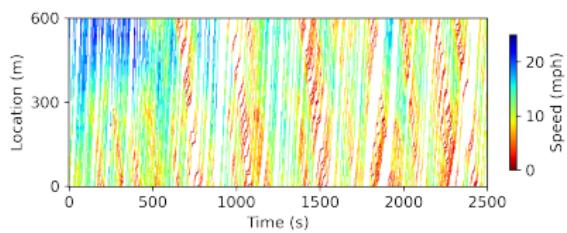


MAPE = 41.40%, RMSE = 1.42mph

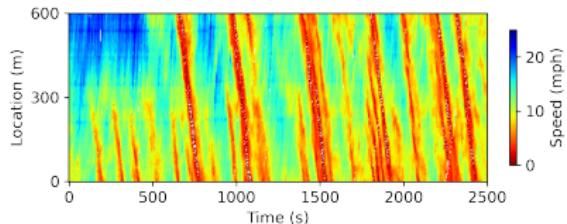


MAPE = 43.97%, RMSE = 1.42mph

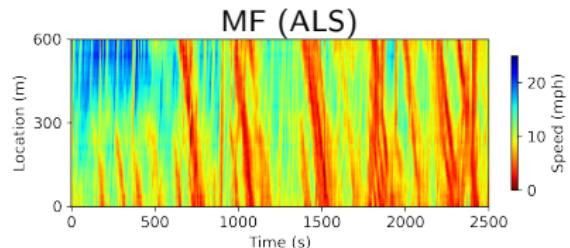
# Which Model Is Better?



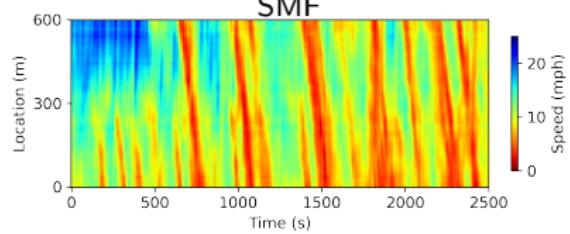
Sparse speed field



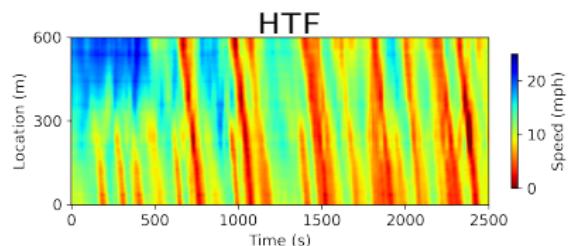
Ground truth speed field



MF (ALS)

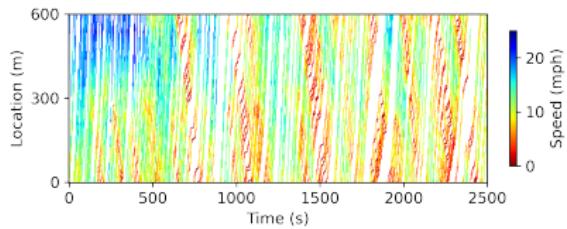


SMF

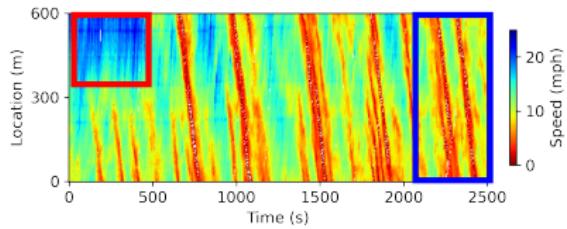


HTF

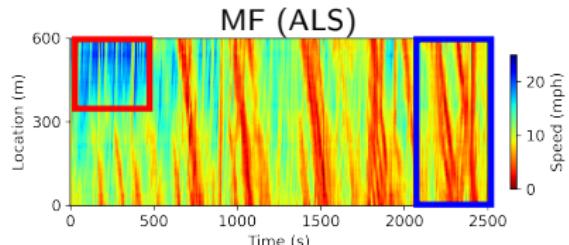
# Which Model Is Better?



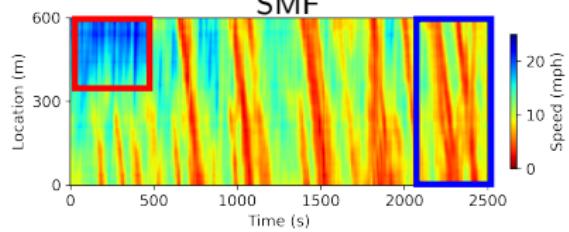
Sparse speed field



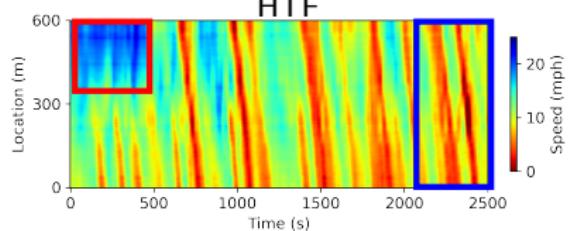
Ground truth speed field



MF (ALS)



SMF



HTF

# Which Model Is Better?

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- Gray image inpainting
  - Randomly mask 90% pixels;
  - MF:  $R = 50$ ,  $\rho = 10^{-1}$ ;
  - SMF:  $R = 50$ ,  $\rho = 10^{-1}$ ,  $\lambda = 10$ .



Incomplete image



MF



SMF



Ground truth



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# Thanks for your attention!

## Any Questions?

### About me:

-  Homepage: <https://xinychen.github.io>
-  GitHub: <https://github.com/xinychen> (3K+ stars)
-  Blog: <https://medium.com/@xinyu.chen> (60K+ views)
-  How to reach me: [chenxy346@gmail.com](mailto:chenxy346@gmail.com)