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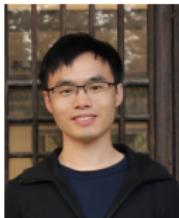
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# Low-Rank Matrix and Tensor Factorization for Speed Field Reconstruction

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McGill University

- 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)

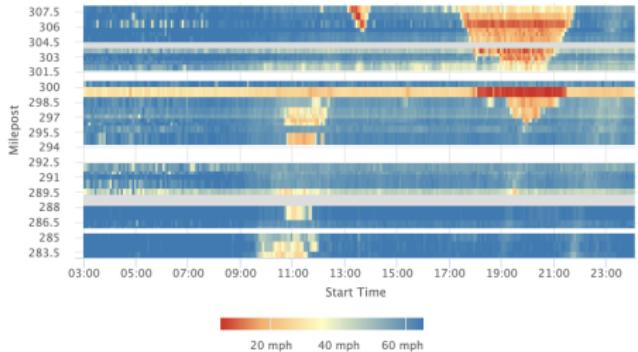
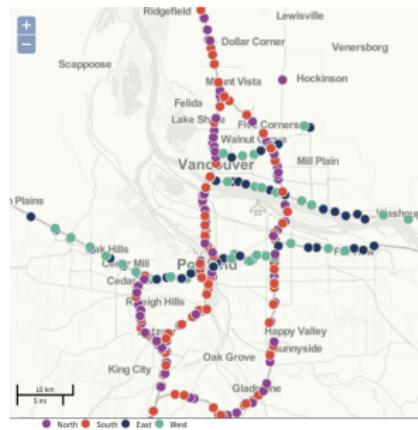
# Outline

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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?
- **Conclusion**

# Motivation

- Portland highway traffic speed data<sup>1</sup>



Traffic speed field

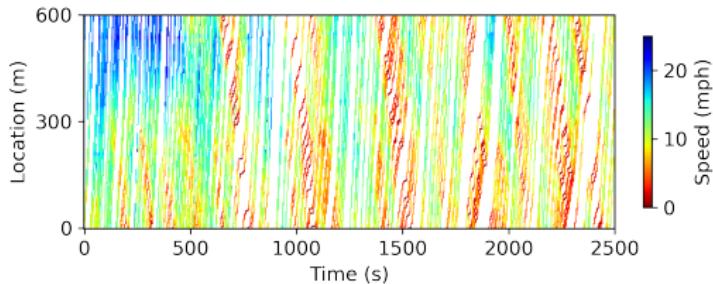
Highway network & sensor locations

- Speed field  $\mathbf{Y} \in \mathbb{R}^{N \times T}$  ( $N$  locations &  $T$  time steps)
- Speed field shows strong spatial/temporal dependencies

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

# Motivation

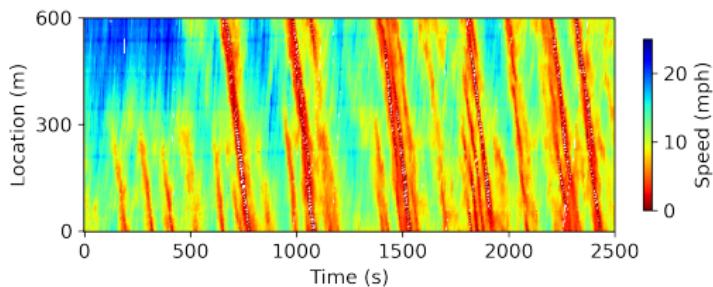
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200-by-500 matrix  
(NGSIM)



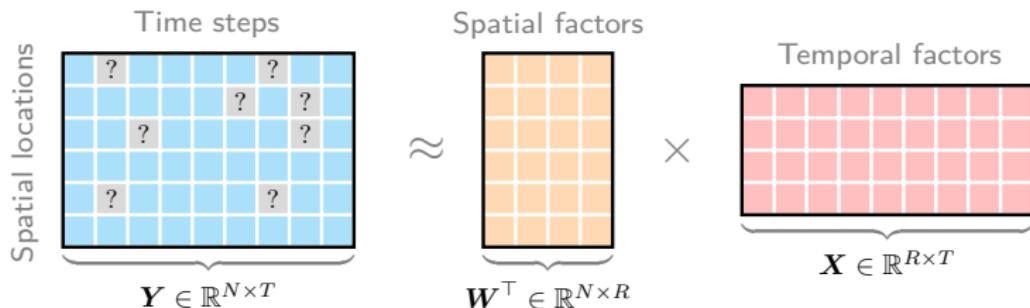
Reconstruct speed field from  
20% sparse trajectories?



- 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!



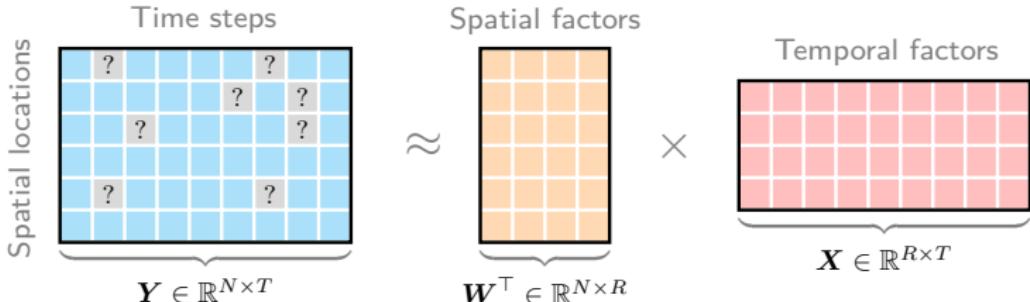
- MF optimization problem

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

with factor matrices  $\mathbf{W}$  and  $\mathbf{X}$ . ( $\|\cdot\|_F^2$  is the squared Frobenius norm.)

- Object 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**)

$$\begin{cases} \frac{\partial f}{\partial \mathbf{W}} = \mathbf{0} \\ \frac{\partial f}{\partial \mathbf{X}} = \mathbf{0} \end{cases} \implies \begin{cases} \mathbf{w}_i := \left( \sum_{t:(i,t) \in \Omega} \mathbf{x}_t \mathbf{x}_t^{\top} + \rho \mathbf{I}_R \right)^{-1} \sum_{t:(i,t) \in \Omega} \mathbf{x}_t y_{i,t} \\ \mathbf{x}_t := \left( \sum_{i:(i,t) \in \Omega} \mathbf{w}_i \mathbf{w}_i^{\top} + \rho \mathbf{I}_R \right)^{-1} \sum_{i:(i,t) \in \Omega} \mathbf{w}_i y_{i,t} \end{cases}$$

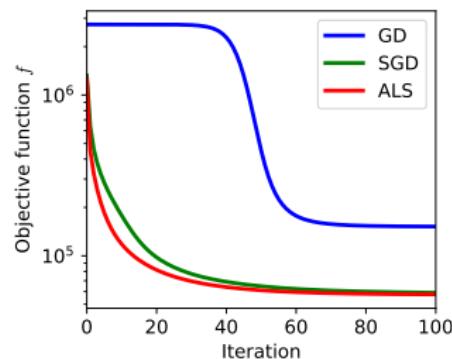
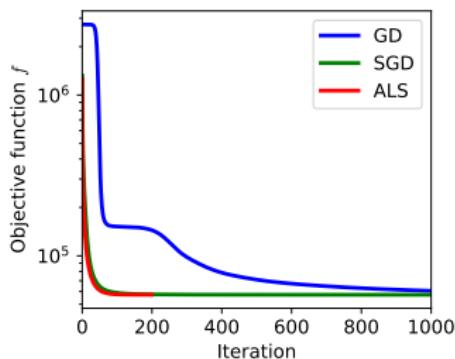
- Latent factors

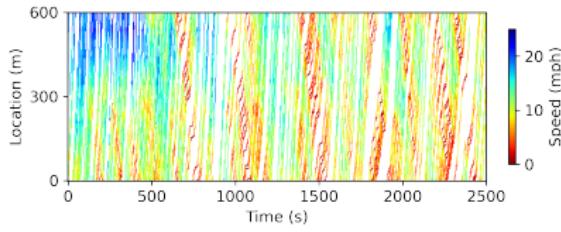
- $\mathbf{w}_i \in \mathbb{R}^R, i = 1, 2, \dots, N$  are the columns of  $\mathbf{W}$ ;
- $\mathbf{x}_t \in \mathbb{R}^R, t = 1, 2, \dots, T$  are the columns of  $\mathbf{X}$ .

# Matrix Factorization

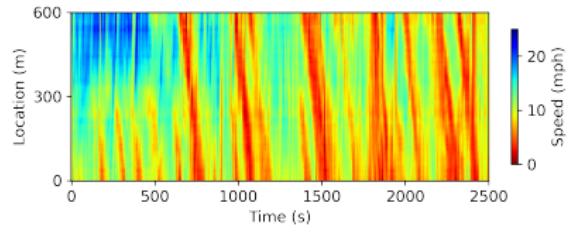
## Speed field reconstruction

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

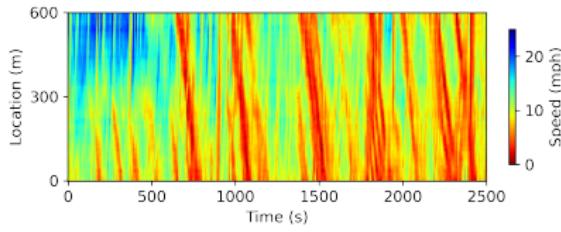




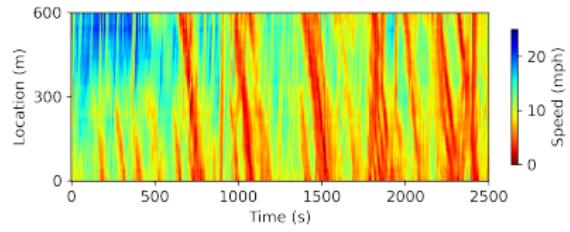
Sparse speed field



MF with GD



MF with SGD



MF with ALS

- Reconstruction errors

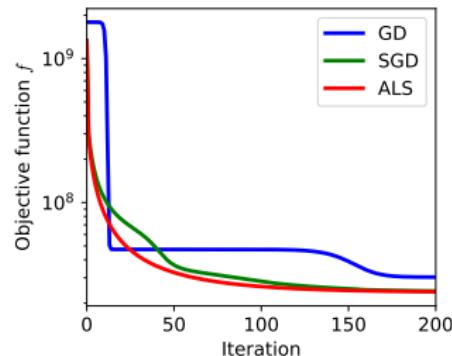
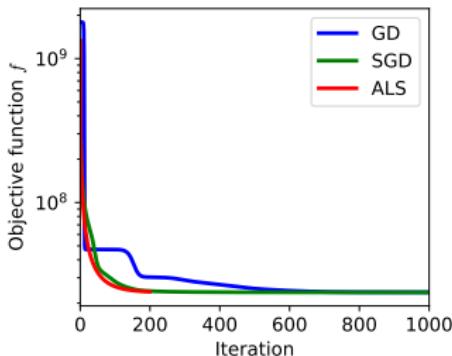
$$\text{MAPE} = \begin{cases} 50.66\% & (\text{GD}) \\ 45.13\% & (\text{SGD}) \\ 45.84\% & (\text{ALS}) \end{cases}$$

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

# Matrix Factorization

**Seattle freeway traffic speed dataset** (randomly mask 60% entries)

- Dataset: 323 loop detectors & 8,064 time steps (288 per day)
- Objective function  $f$  vs. iteration
  - Set rank  $R = 10$ , weight parameter  $\rho = 10^2$ ;
  - Set GD step size  $\alpha = 2 \times 10^{-5}$ .



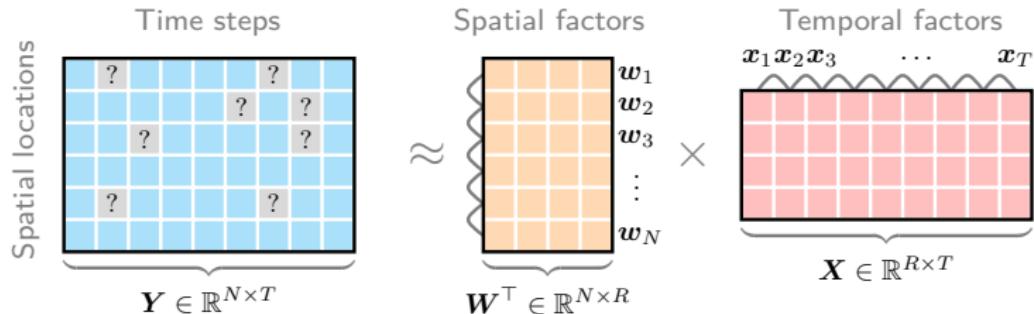
- Reconstruction errors

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

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

# 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

$$\Psi = \begin{bmatrix} -1 & 1 & 0 & \cdots & 0 & 0 \\ 0 & -1 & 1 & \cdots & 0 & 0 \\ 0 & 0 & -1 & \cdots & 0 & 0 \\ \vdots & \vdots & \vdots & \ddots & \vdots & \vdots \\ 0 & 0 & 0 & \cdots & -1 & 1 \end{bmatrix} \implies \begin{cases} \|\mathbf{W}\boldsymbol{\Psi}_1^\top\|_F^2 & \text{with } \boldsymbol{\Psi}_1 \in \mathbb{R}^{(N-1) \times N} \\ \|\mathbf{X}\boldsymbol{\Psi}_2^\top\|_F^2 & \text{with } \boldsymbol{\Psi}_2 \in \mathbb{R}^{(T-1) \times T} \end{cases}$$

- SMF optimization problem

$$\begin{aligned} \min_{\mathbf{W}, \mathbf{X}} \quad & \frac{1}{2} \left\| \mathcal{P}_\Omega(\mathbf{Y} - \mathbf{W}^\top \mathbf{X}) \right\|_F^2 + \frac{\rho}{2} (\|\mathbf{W}\|_F^2 + \|\mathbf{X}\|_F^2) \\ & + \frac{\lambda}{2} (\|\mathbf{W}\boldsymbol{\Psi}_1^\top\|_F^2 + \|\mathbf{X}\boldsymbol{\Psi}_2^\top\|_F^2) \end{aligned}$$

- **Alternating minimization**

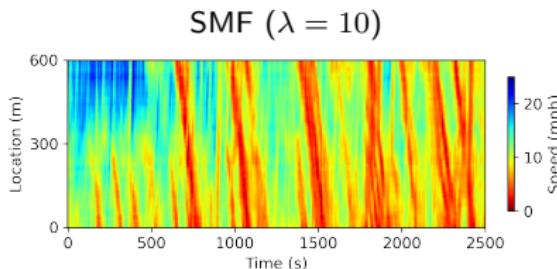
$$\mathbf{W} := \{ \mathbf{W} \mid \frac{\partial f}{\partial \mathbf{W}} = \mathbf{0} \} \quad \mathbf{X} := \{ \mathbf{X} \mid \frac{\partial f}{\partial \mathbf{X}} = \mathbf{0} \}$$

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

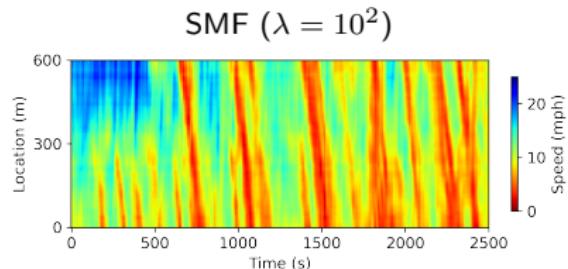
# Smoothing Matrix Factorization

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

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



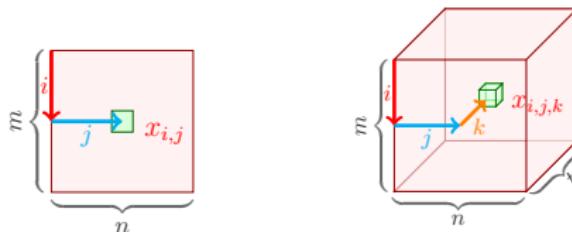
MAPE = 44.06%, RMSE = 2.16mph



MAPE = 48.00%, RMSE = 1.60mph

# Tensor Factorization

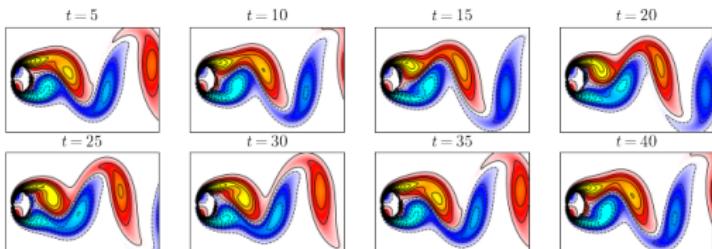
- What is tensor?  $\mathbf{X} \in \mathbb{R}^{m \times n}$  vs.  $\mathcal{X} \in \mathbb{R}^{m \times n \times t}$



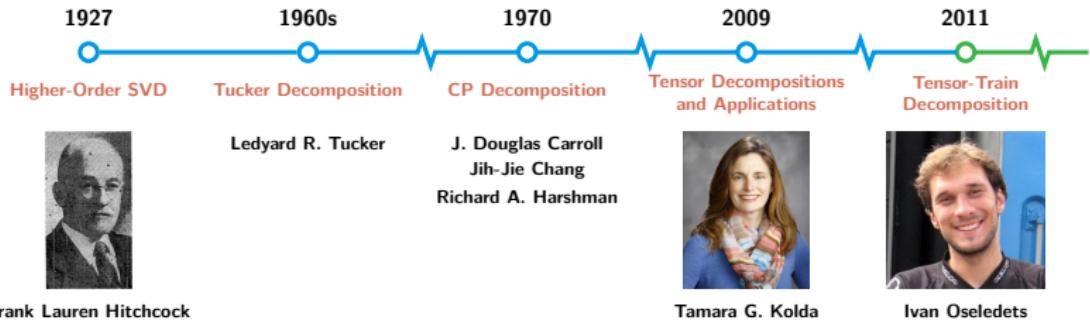
- Tensors are everywhere!



Color image with  
RGB channels

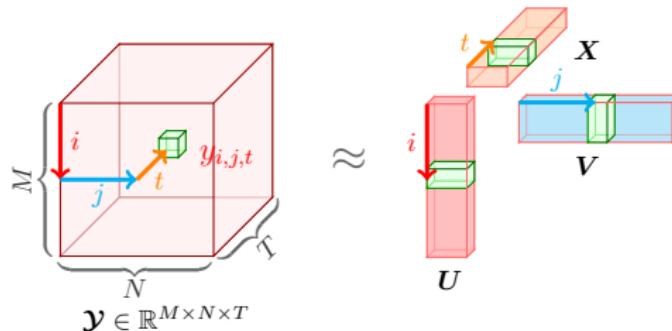


Dynamical system (fluid flow)



# 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>2,3</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>2</sup>CANDECOMP/PARAFAC (CP) decomposition.

<sup>3</sup>The symbol  $\otimes$  denotes the outer product.

# Hankel Tensor and Its Factorization

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- Hankel matrix

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

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

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

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

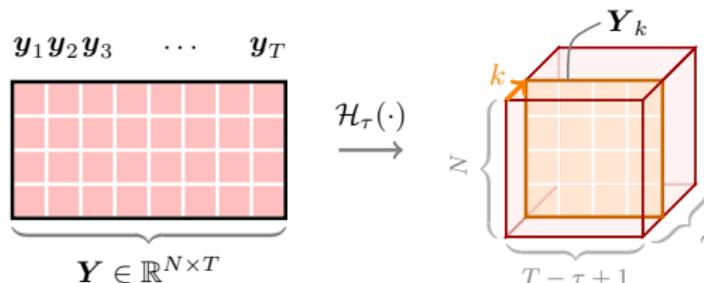
$$\implies \hat{\mathbf{y}} = \begin{bmatrix} \hat{y}_1 \\ \hat{y}_2 \\ \hat{y}_3 \\ \hat{y}_4 \\ \hat{y}_5 \end{bmatrix} = \mathcal{H}_\tau^{-1} \left( \begin{bmatrix} v_1 x_1 & v_1 x_2 \\ v_2 x_1 & v_2 x_2 \\ v_3 x_1 & v_3 x_2 \\ v_4 x_1 & v_4 x_2 \end{bmatrix} \right) = \begin{bmatrix} v_1 x_1 \\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

- Automatic temporal modeling.

# Hankel Tensor and Its Factorization

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

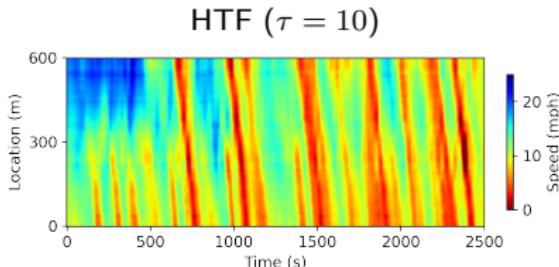


# Hankel Tensor and Its Factorization

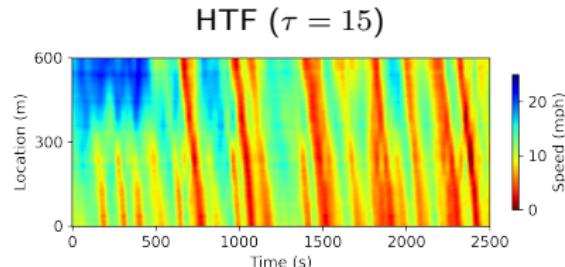
- HTF optimization problem

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

- 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.

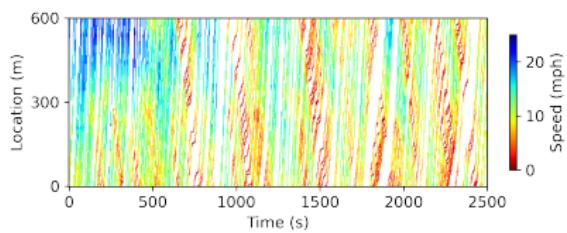


MAPE = 41.40%, RMSE = 1.42mph

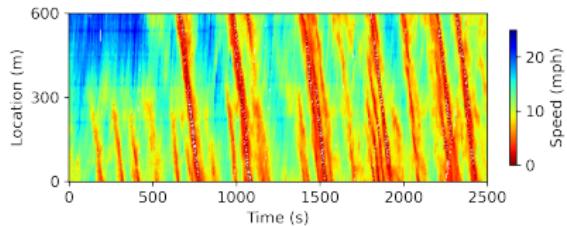


MAPE = 43.97%, RMSE = 1.42mph

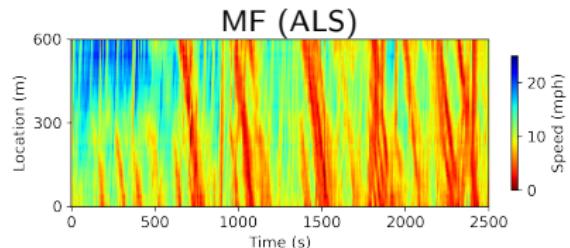
# Which Model Is Better?



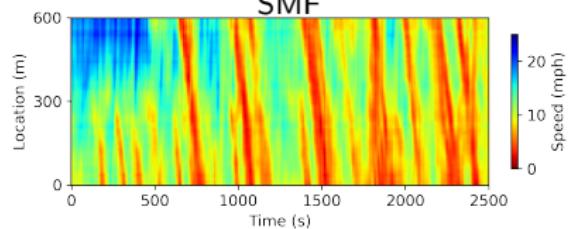
Sparse speed field



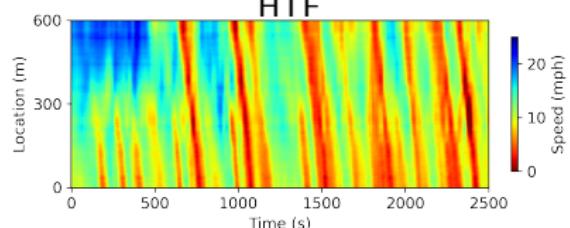
Ground truth speed field



MF (ALS)

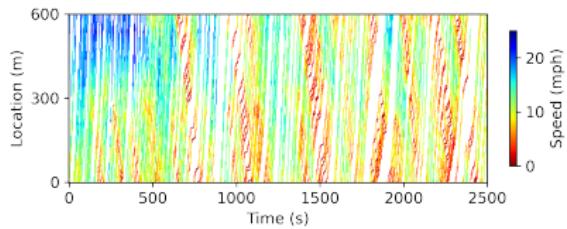


SMF

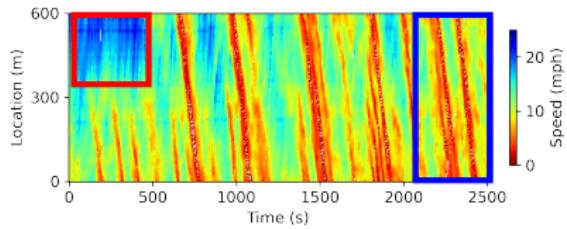


HTF

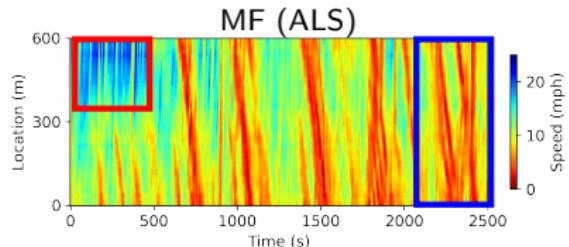
# Which Model Is Better?



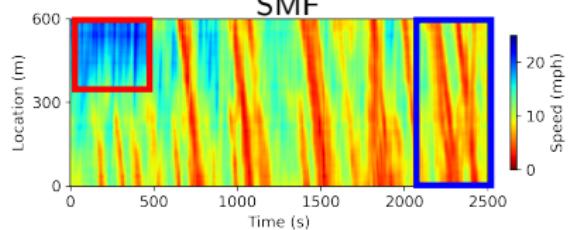
Sparse speed field



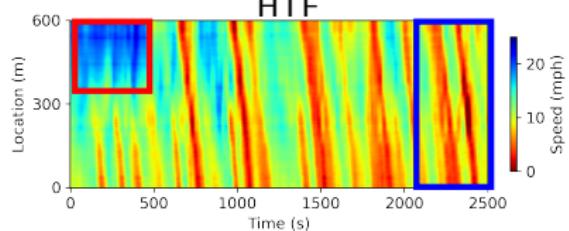
Ground truth speed field



MF (ALS)



SMF



HTF

## Which Model Is Better?

---

- Seattle freeway traffic speed data
  - Randomly mask 60% entries;
  - SMF: set  $R = 10$ ,  $\rho = 10^2$ ,  $\lambda = 2 \times 10^2$ ;
  - HTF: set  $\tau = 6$ ,  $R = 10$ ,  $\rho = 10^2$ ;
  - Reconstruction errors

$$\text{MAPE} = \begin{cases} 9.13\% & (\text{MF}) \\ 9.01\% & (\text{SMF}) \\ \mathbf{8.67\%} & (\text{HTF}) \end{cases} \quad \text{RMSE} = \begin{cases} 5.24 & (\text{MF}) \\ 5.14 & (\text{SMF}) \text{ (mph)} \\ \mathbf{5.02} & (\text{HTF}) \end{cases}$$

# Which Model Is Better?

---

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



Incomplete image



MF



SMF



Ground truth

# Conclusion

---

- How to reconstruct sparse speed field?
  - ✓ Matrix factorization (**MF**)   ✓ Tensor factorization (**TF**)
- The importance of spatiotemporal modeling in low-rank methods?
  - Spatial/temporal **smoothing** regularization:

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

- Automatic temporal modeling via **Hankelization**:

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



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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)
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