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IVADO

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
2. **Jupyter Notebook**: https://github.com/xinychen/transdim/blob/master/toy-examples/MF_TF_SFR.ipynb

Outline

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Motivation

Motivation

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

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

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

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

Matrix Factorization

- MF optimization problem

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

- Orthogonal projection $\mathcal{P}_\Omega : \mathbb{R}^{N \times T} \to \mathbb{R}^{N \times T}$?
  - Simple example: $\boldsymbol{Y} = \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}$ with $\Omega = \{(1,1),(2,2)\}$, we have

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

- Role of regularization (with ρ): avoid overfitting.

Matrix Factorization

- MF optimization problem

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

- Partial derivatives

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

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

$$\begin{cases} \boldsymbol{W} := \boldsymbol{W} - \alpha\dfrac{\partial f}{\partial \boldsymbol{W}} \\ \boldsymbol{X} := \boldsymbol{X} - \alpha\dfrac{\partial f}{\partial \boldsymbol{X}} \end{cases} \quad \text{vs.} \quad \begin{cases} \alpha := \arg\min\limits_{\alpha} \ f(\boldsymbol{W} - \alpha\dfrac{\partial f}{\partial \boldsymbol{W}}, \boldsymbol{X}) \\ \boldsymbol{W} := \boldsymbol{W} - \alpha\dfrac{\partial f}{\partial \boldsymbol{W}} \\ \beta := \arg\min\limits_{\beta} \ f(\boldsymbol{W}, \boldsymbol{X} - \beta\dfrac{\partial f}{\partial \boldsymbol{X}}) \\ \boldsymbol{X} := \boldsymbol{X} - \beta\dfrac{\partial f}{\partial \boldsymbol{X}} \end{cases}$$

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

Matrix Factorization

- MF optimization problem

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

- Partial derivatives

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

- Alternating least squares (**ALS**)

$$\begin{cases} \boldsymbol{w}_i := \Big(\sum\limits_{t:(i,t)\in\Omega} \boldsymbol{x}_t\boldsymbol{x}_t^\top + \rho\boldsymbol{I}_R\Big)^{-1} \sum\limits_{t:(i,t)\in\Omega} \boldsymbol{x}_t y_{i,t} \\ \boldsymbol{x}_t := \Big(\sum\limits_{i:(i,t)\in\Omega} \boldsymbol{w}_i\boldsymbol{w}_i^\top + \rho\boldsymbol{I}_R\Big)^{-1} \sum\limits_{i:(i,t)\in\Omega} \boldsymbol{w}_i y_{i,t} \end{cases}$$

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

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

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

Matrix Factorization

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

- 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

$$\text{MAPE} = \begin{cases} 9.14\% & \text{(GD)} \\ 9.12\% & \text{(SGD)} \\ 9.13\% & \text{(ALS)} \end{cases} \qquad \text{RMSE} = \begin{cases} 5.24 & \text{(GD)} \\ 5.24 & \text{(SGD)} \\ 5.24 & \text{(ALS)} \end{cases} \quad \text{(mph)}$$

Smoothing Matrix Factorization

- Spatial/temporal local dependencies are also important!

- Formulate spatial/temporal dependencies

$$\boldsymbol{W}\boldsymbol{\Psi}_1^\top = \begin{bmatrix} | & & | \\ \boldsymbol{w}_2 - \boldsymbol{w}_1 & \cdots & \boldsymbol{w}_N - \boldsymbol{w}_{N-1} \\ | & & | \end{bmatrix}$$

$$\boldsymbol{X}\boldsymbol{\Psi}_2^\top = \begin{bmatrix} | & & | \\ \boldsymbol{x}_2 - \boldsymbol{x}_1 & \cdots & \boldsymbol{x}_T - \boldsymbol{x}_{T-1} \\ | & & | \end{bmatrix}$$

Smoothing Matrix Factorization

- Formulate spatial/temporal dependencies

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

- SMF optimization problem

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

- **Alternating minimization**

$$\boldsymbol{W} := \{\boldsymbol{W} \mid \frac{\partial f}{\partial \boldsymbol{W}} = \boldsymbol{0}\} \qquad \boldsymbol{X} := \{\boldsymbol{X} \mid \frac{\partial f}{\partial \boldsymbol{X}} = \boldsymbol{0}\}$$

- Solving 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:

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

SMF ($\lambda = 10$)

MAPE = **44.06%**, RMSE = 2.16mph

SMF ($\lambda = 10^2$)

MAPE = 48.00%, RMSE = **1.60mph**

Tensor Factorization

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

- Real-world tensors

Color image with RGB channels

Dynamical system (fluid flow)

1927 — Higher-Order SVD

Frank Lauren Hitchcock

1960s — Tucker Decomposition

Ledyard R. Tucker

1970 — CP Decomposition

J. Douglas Carroll
Jih-Jie Chang
Richard A. Harshman

2009 — Tensor Decompositions and Applications

Tamara G. Kolda

2011 — Tensor-Train Decomposition

Ivan Oseledets

CP Tensor Factorization

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

- Understanding CP factorization[1]:

$$\begin{cases} y_{i,j,t} \approx \sum_{r=1}^{R} u_{i,r} v_{j,r} x_{t,r} & \text{(sum of latent factors)} \\ \mathcal{Y} \approx \sum_{r=1}^{R} \boldsymbol{u}_r \otimes \boldsymbol{v}_r \otimes \boldsymbol{x}_r & \text{(sum of rank-one tensors)} \end{cases}$$

[1] The symbol $\otimes$ denotes the outer product.

Hankel Tensor and Its Factorization

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

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

  - On time series?
- (Hankelization) Hankel tensor $\mathcal{H}_\tau(\boldsymbol{Y})$
  - Tensor size: $N \times (T - \tau + 1) \times \tau$;
  - Slices: $\boldsymbol{Y}_k = \begin{bmatrix} | & | & & | \\ \boldsymbol{y}_k & \boldsymbol{y}_{k+1} & \cdots & \boldsymbol{y}_{T-\tau+k} \\ | & | & & | \end{bmatrix}$, $k = 1, 2, \ldots, \tau$;
  - Slice size: $N \times (T - \tau + 1)$.

Hankel Tensor and Its Factorization

- HTF optimization problem

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

- 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.

HTF ($\tau = 10$)

MAPE = **41.40%**, RMSE = **1.42mph**

HTF ($\tau = 15$)

MAPE = 43.97%, RMSE = **1.42mph**

Which Model Is Better?

Sparse speed field

Ground truth speed field

Which Model Is Better?

Sparse speed field

Ground truth speed field

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

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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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