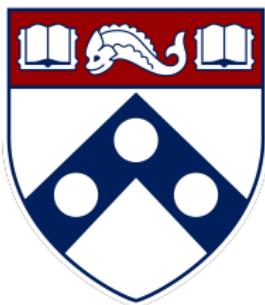


## **Tensor decomposition and completion**



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Wharton Statistics & Data Science, Spring 2022

# Outline

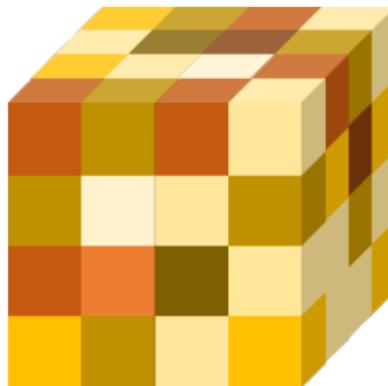
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- Tensor decomposition
- Latent variable models & tensor decomposition
- Tensor power method
- Tensor completion

# **Tensor decomposition**

# Tensor

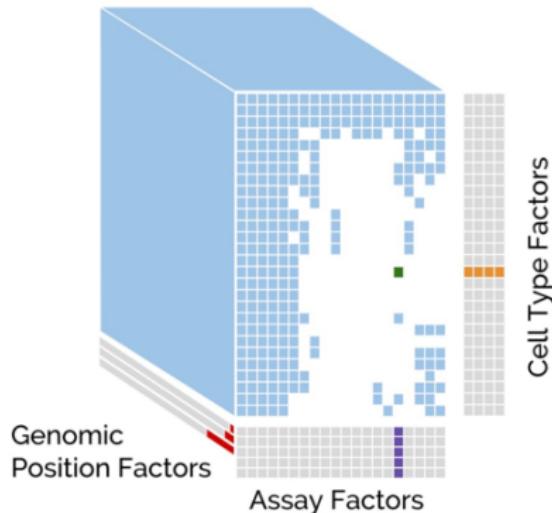
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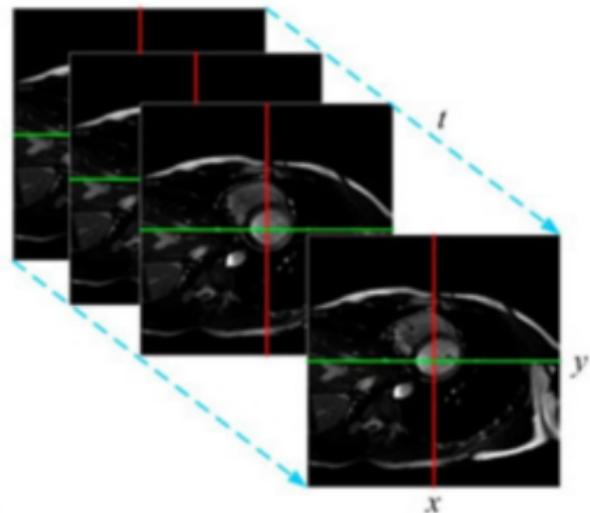
An order- $d$  tensor  $\mathbf{T} = [T_{i_1, \dots, i_d}]_{1 \leq i_1, \dots, i_d \leq n}$  is a  $d$ -way array

- a matrix is a tensor of order 2

# Ubiquity of high-dimensional tensor data



computational genomics  
— *fig. credit: Schreiber et al. 19*



dynamic MRI  
— *fig. credit: Liu et al. 17*

# Basics

---

- **Rank-1 tensor:**  $\mathbf{T} = \mathbf{x} \otimes \mathbf{x} \otimes \mathbf{x}$  denotes a tensor such that

$$T_{i_1, \dots, i_d} = x_{i_1} x_{i_2} \cdots x_{i_d}$$

- inner product of two tensors  $\mathbf{T}$  and  $\mathbf{A}$ :

$$\langle \mathbf{T}, \mathbf{A} \rangle := \sum_{i_1, \dots, i_d} T_{i_1, \dots, i_d} A_{i_1, \dots, i_d}$$

- Frobenius norm of a tensor  $\mathbf{T}$ :

$$\|\mathbf{T}\|_{\text{F}} := \sqrt{\sum_{i_1, \dots, i_d} T_{i_1, \dots, i_d}^2}$$

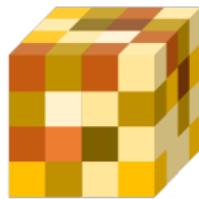
- operator norm of an order- $d$  tensor  $\mathbf{T}$ :

$$\|\mathbf{T}\| = \max_{\{\mathbf{u}_i\}: \|\mathbf{u}_i\|_2=1} \langle \mathbf{T}, \mathbf{u}_1 \otimes \cdots \otimes \mathbf{u}_d \rangle$$

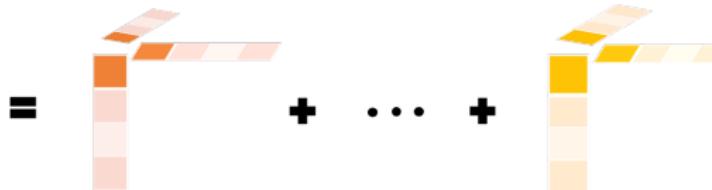
# Tensor decomposition

Suppose we observe an order- $d$  tensor

$$\mathbf{T} = \sum_{i=1}^r \lambda_i \mathbf{u}_i \otimes \mathbf{u}_i \otimes \cdots \otimes \mathbf{u}_i$$



true tensor



rank-1 tensor

rank-1 tensor

**Question:** can we recover  $\{\mathbf{u}_i\}$  and  $\{\lambda_i\}$  given  $\mathbf{T}$ ?

- if  $d = 2$  (matrix case), it is often not recoverable; what if  $d \geq 3$ ?
- this question arises in a number of latent-variable models

# **Latent variable models and tensor decomposition**

# Notation

---

- probability simplex

$$\Delta_n := \{z \in \mathbb{R}^n \mid z_i \geq 0, \forall i; \mathbf{1}^\top z = 1\}$$

- any vector  $w \in \Delta_n$  represents a distribution (or probability mass function) over  $n$  objects

# A simple topic model

---

Consider a collection of documents

- $r$ : the number of distinct topics
- $n$ : the number of distinct words in vocabulary

# A simple topic model

---

Consider a collection of documents

- each time, draw 3 words as follows

- pick  $\underbrace{\text{a topic } h}_{\text{latent variable}}$  according to distribution  $[w_1, \dots, w_r] \in \Delta_r$  s.t.

$$\mathbb{P}\{h = j\} = w_j, \quad 1 \leq j \leq r$$

- given topic  $h$ , draw 3 independent words from this topic according to the distribution

$$\underbrace{\mu_h}_{\text{determined only by the topic}} \in \Delta_n$$

**Goal:** recover  $\{\mu_i\}$  and  $\{w_i\}$  from the collected samples

## Moment method for the topic model

---

Denote the 3 words we draw as  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)} \in \mathbb{R}^n$ :

$$\mathbf{x}^{(i)} = \mathbf{e}_j \quad \text{if the } i\text{th word is } j$$

It is straightforward to check

$$\mathbf{M}_2 := \mathbb{E}[\mathbf{x}^{(1)} \otimes \mathbf{x}^{(2)}] = \sum_{i=1}^r w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$$

$$\mathbf{M}_3 := \mathbb{E}[\mathbf{x}^{(1)} \otimes \mathbf{x}^{(2)} \otimes \mathbf{x}^{(3)}] = \sum_{i=1}^r w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$$

- $\mathbf{M}_2, \mathbf{M}_3$  can be reliably estimated when we have many samples
- recovering  $\{\boldsymbol{\mu}_i\}$  and  $\{w_i\}$  from  $\mathbf{M}_2, \mathbf{M}_3$   
 $\iff$  tensor decomposition

## Latent Dirichlet allocation (LDA)

---

More complicated topic models: **mixed membership models**, where each data might belong to multiple latent classes simultaneously

This means: the latent variable  $h$  is no longer an indicator of topics, but rather, a topic mixture  $\mathbf{h} \in \Delta_r$

# Latent Dirichlet allocation (LDA)

---

- $n$ : the number of distinct words in the vocabulary
- $r$ : the number of distinct topics
- topic  $i$  has word distribution  $\mu_i \in \Delta_n$  ( $1 \leq i \leq n$ )
- each time, draw 3 words as follows
  - draw  $\underbrace{\text{topic mixture } \mathbf{h}}_{\text{latent variables}} \in \Delta_r$  according to Dirichlet distribution

$$p_{\alpha}(\mathbf{h}) = \frac{\Gamma(\alpha_0)}{\prod_{i=1}^r \Gamma(\alpha_i)} \prod_{i=1}^r h_i^{\alpha_i - 1}$$

- draw  $\mathbf{x}^{(1)}, \mathbf{x}^{(2)}, \mathbf{x}^{(3)} \in \mathbb{R}^n$  independently according to the *mixed distribution*  $\sum_{i=1}^r h_i \mu_i$

# Moment method for latent Dirichlet allocation

---

$$\mathbf{M}_1 := \mathbb{E}[\mathbf{x}^{(1)}]$$

$$\mathbf{M}_2 := \mathbb{E}[\mathbf{x}^{(1)} \otimes \mathbf{x}^{(2)}] - \frac{\alpha_0}{\alpha_0 + 1} \mathbf{M}_1 \otimes \mathbf{M}_1 = \sum_{i=1}^r \frac{\alpha_i}{(\alpha_0 + 1)\alpha_0} \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$$

$$\mathbf{M}_3 := \mathbb{E}[\mathbf{x}^{(1)} \otimes \mathbf{x}^{(2)} \otimes \mathbf{x}^{(3)}] - \frac{\alpha_0}{\alpha_0 + 2}$$

$$\cdot \left( \mathbb{E}[\mathbf{x}^{(1)} \otimes \mathbf{x}^{(2)} \otimes \mathbf{M}_1] + \mathbb{E}[\mathbf{x}^{(1)} \otimes \mathbf{M}_1 \otimes \mathbf{x}^{(2)}] + \mathbb{E}[\mathbf{M}_1 \otimes \mathbf{x}^{(1)} \otimes \mathbf{x}^{(2)}] \right)$$

$$+ \frac{2\alpha_0^2}{(\alpha_0 + 2)(\alpha_0 + 1)} \mathbf{M}_1 \otimes \mathbf{M}_1 \otimes \mathbf{M}_1$$

$$= \sum_{i=1}^r \frac{2\alpha_i}{(\alpha_0 + 2)(\alpha_0 + 1)\alpha_0} \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$$

- estimate  $\mathbf{M}_1, \mathbf{M}_2, \mathbf{M}_3$  from samples (assuming  $\alpha_0$  is known)
- recover  $\{\boldsymbol{\mu}_i\}$  and  $\{\alpha_i\}_{i \geq 1}$  from  $\mathbf{M}_2, \mathbf{M}_3$  (tensor decomposition)

# Gaussian mixture model

---

- $r$  Gaussian distributions  $\mathcal{N}(\boldsymbol{\mu}_i, \sigma^2 \mathbf{I}_n)$  ( $1 \leq i \leq r$ )
- a sample  $\mathbf{x} \in \mathbb{R}^n$  is drawn as follows
  - the latent indicator variable  $h$  is generated according to distribution  $[w_1, \dots, w_r] \in \Delta_r$  s.t.

$$\mathbb{P}(h = i) = w_i, \quad 1 \leq i \leq r$$

- generate  $\mathbf{x}$  from  $\mathcal{N}(\boldsymbol{\mu}_h, \sigma^2 \mathbf{I}_n)$

## Moment method for Gaussian mixture model

---

$$\boldsymbol{M}_2 := \mathbb{E}[\boldsymbol{x} \otimes \boldsymbol{x}] - \sigma^2 \boldsymbol{I} = \sum_{i=1}^r w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i$$

$$\boldsymbol{M}_3 := \mathbb{E}[\boldsymbol{x} \otimes \boldsymbol{x} \otimes \boldsymbol{x}]$$

$$\begin{aligned} & - \sigma^2 \sum_{i=1}^n (\mathbb{E}[\boldsymbol{x}] \otimes \boldsymbol{e}_i \otimes \boldsymbol{e}_i + \boldsymbol{e}_i \otimes \mathbb{E}[\boldsymbol{x}] \otimes \boldsymbol{e}_i + \boldsymbol{e}_i \otimes \boldsymbol{e}_i \otimes \mathbb{E}[\boldsymbol{x}]) \\ & = \sum_{i=1}^r w_i \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \otimes \boldsymbol{\mu}_i \end{aligned}$$

- $\boldsymbol{M}_2$ ,  $\boldsymbol{M}_3$  and  $\mathbb{E}[\boldsymbol{x}]$  can all be reliably estimated when there are many samples
- recover  $\{\boldsymbol{\mu}_i\}$  and  $\{w_i\}$  from  $\boldsymbol{M}_2$ ,  $\boldsymbol{M}_3$  (tensor decomposition)

## **Tensor power method**

# Main task

---

Given

$$\mathbf{M}_2 = \sum_{i=1}^r \lambda_i \mathbf{u}_i \otimes \mathbf{u}_i$$

$$\mathbf{M}_3 = \sum_{i=1}^r \lambda_i \mathbf{u}_i \otimes \mathbf{u}_i \otimes \mathbf{u}_i$$

where  $\lambda_i > 0$

**Question:** can we recover  $\{\lambda_i\}$  and  $\{\mathbf{u}_i\}$  from  $\mathbf{M}_2$  and  $\mathbf{M}_3$ ?

## An easier case: orthogonal decomposition

---

Given

$$M_2 = \sum_{i=1}^r \lambda_i \mathbf{u}_i \otimes \mathbf{u}_i$$

$$M_3 = \sum_{i=1}^r \lambda_i \mathbf{u}_i \otimes \mathbf{u}_i \otimes \mathbf{u}_i$$

where  $\lambda_i > 0$ ,  $r \leq n$ , and  $\{\mathbf{u}_i\}$  are orthonormal

**Question:** can we recover  $\{\lambda_i\}$  and  $\{\mathbf{u}_i\}$  from  $M_2$  and  $M_3$ ?

## Tensor power method

## Define

$$\mathbf{T}(\mathbf{I}, \mathbf{x}, \dots, \mathbf{x}) \coloneqq \sum_{i=1}^r \lambda_i (\mathbf{u}_i^\top \mathbf{x})^{d-1} \mathbf{u}_i$$

- if  $d = 2$  (matrix case):  $\mathbf{T}(\mathbf{I}, \mathbf{x}) = \mathbf{T}\mathbf{x}$

**Algorithm 5.1** Tensor power method

- ```

1: initialize  $\mathbf{x}_0 \leftarrow$  random unit vector
2: for  $t = 1, 2, \dots$  do
3:    $\mathbf{x}_t = \mathbf{T}(\mathbf{I}, \mathbf{x}_{t-1}, \dots, \mathbf{x}_{t-1})$  (power iteration)
4:    $\mathbf{x}_t \leftarrow \frac{1}{\|\mathbf{x}_t\|_2} \mathbf{x}_t$  (re-normalization)

```

# Convergence analysis

## Theorem 5.1 (Convergence of tensor power method)

Suppose  $\{\mathbf{u}_i\}$  are orthonormal,  $\lambda_i > 0$  ( $1 \leq i \leq r$ ),  $r \leq n$ , and  $d = 3$ . Then for any  $1 \leq i \leq r$ ,

$$1 - \frac{(\mathbf{u}_i^\top \mathbf{x}_t)^2}{\|\mathbf{x}_t\|_2^2} \leq \lambda_i^2 \sum_{j:j \neq i} \lambda_j^{-2} \left( \frac{\lambda_j \mathbf{u}_j^\top \mathbf{x}_0}{\lambda_i \mathbf{u}_i^\top \mathbf{x}_0} \right)^{2^{t+1}}$$

- tensor power method converges quadratically to some  $\mathbf{u}_i$
- it converges to a point  $\mathbf{u}_i$  associated with the largest  $\lambda_i \mathbf{u}_i^\top \mathbf{x}_0$ 
  - both the eigenvalue and the initial point matter!

## Proof of Theorem 5.1

---

Note that removing “re-normalization” steps does not affect  $\frac{(\mathbf{u}_i^\top \mathbf{x}_t)^2}{\|\mathbf{x}_t\|_2^2}$  at all. For simplicity, we assume

$$\mathbf{x}_t = \mathbf{T}(\mathbf{I}, \mathbf{x}_{t-1}, \mathbf{x}_{t-1}) = \sum_{i=1}^r \lambda_i (\mathbf{u}_i^\top \mathbf{x}_{t-1})^2 \mathbf{u}_i$$

Observe that

- since  $\mathbf{x}_1 = \sum_{i=1}^r \lambda_i (\mathbf{u}_i^\top \mathbf{x}_0)^2 \mathbf{u}_i$ , we have

$$(\mathbf{u}_i^\top \mathbf{x}_1)^2 = \lambda_i^2 (\mathbf{u}_i^\top \mathbf{x}_0)^4$$

- since  $\mathbf{x}_2 = \sum_{i=1}^r \lambda_i (\mathbf{u}_i^\top \mathbf{x}_1)^2 \mathbf{u}_i$ , we have

$$(\mathbf{u}_i^\top \mathbf{x}_2)^2 = \lambda_i^2 (\mathbf{u}_i^\top \mathbf{x}_1)^4 = \lambda_i^6 (\mathbf{u}_i^\top \mathbf{x}_0)^8$$

- since  $\mathbf{x}_3 = \sum_{i=1}^r \lambda_i (\mathbf{u}_i^\top \mathbf{x}_2)^2 \mathbf{u}_i$ , we have

$$(\mathbf{u}_i^\top \mathbf{x}_3)^2 = \lambda_i^2 (\mathbf{u}_i^\top \mathbf{x}_2)^4 = \lambda_i^{14} (\mathbf{u}_i^\top \mathbf{x}_0)^{16}$$

## Proof of Theorem 5.1 (cont.)

---

By induction, one has

$$(\mathbf{u}_i^\top \mathbf{x}_t)^2 = \lambda_i^{2^{t+1}-2} (\mathbf{u}_i^\top \mathbf{x}_0)^{2^{t+1}}, \quad 1 \leq i \leq r$$

This implies

$$\frac{(\mathbf{u}_i^\top \mathbf{x}_t)^2}{\|\mathbf{x}_t\|_2^2} = \frac{(\mathbf{u}_i^\top \mathbf{x}_t)^2}{\sum_{j=1}^r (\mathbf{u}_j^\top \mathbf{x}_t)^2} = \frac{(\lambda_i \mathbf{u}_i^\top \mathbf{x}_0)^{2^{t+1}}}{\sum_{j=1}^r \left(\frac{\lambda_i}{\lambda_j}\right)^2 (\lambda_j \mathbf{u}_j^\top \mathbf{x}_0)^{2^{t+1}}}$$

and hence

$$\begin{aligned} 1 - \frac{(\mathbf{u}_i^\top \mathbf{x}_t)^2}{\|\mathbf{x}_t\|_2^2} &= \frac{\sum_{j:j \neq i} \left(\frac{\lambda_i}{\lambda_j}\right)^2 (\lambda_j \mathbf{u}_j^\top \mathbf{x}_0)^{2^{t+1}}}{\sum_j \left(\frac{\lambda_i}{\lambda_j}\right)^2 (\lambda_j \mathbf{u}_j^\top \mathbf{x}_0)^{2^{t+1}}} \\ &\leq \frac{\sum_{j:j \neq i} \left(\frac{\lambda_i}{\lambda_j}\right)^2 (\lambda_j \mathbf{u}_j^\top \mathbf{x}_0)^{2^{t+1}}}{(\lambda_i \mathbf{u}_i^\top \mathbf{x}_0)^{2^{t+1}}} \\ &= \lambda_i^2 \sum_{j:j \neq i} \lambda_j^{-2} \left(\frac{\lambda_j \mathbf{u}_j^\top \mathbf{x}_0}{\lambda_i \mathbf{u}_i^\top \mathbf{x}_0}\right)^{2^{t+1}} \end{aligned}$$

## General case: reduction to orthogonally decomposable tensors

---

Suppose  $r \leq n$ , but  $\{\mathbf{u}_i\}$  are not orthonormal

**Key idea:** use  $M_2$  to find a “whitening matrix” that allows us to orthogonalize  $\{\mathbf{u}_i\}$

## General case: reduction to orthogonally decomposable tensor

---

Let  $\mathbf{W}$  be a whitening matrix (e.g.  $\mathbf{W} = \mathbf{U}\Lambda^{-1/2}$ ) obeying

$$\mathbf{W}^\top \mathbf{M}_2 \mathbf{W} = \mathbf{I} \quad (5.1)$$

Then

$$\begin{aligned} \mathbf{M}_3(\mathbf{W}, \mathbf{W}, \mathbf{W}) &= \sum_{i=1}^r \lambda_i (\mathbf{W}^\top \mathbf{u}_i) \otimes (\mathbf{W}^\top \mathbf{u}_i) \otimes (\mathbf{W}^\top \mathbf{u}_i) \\ &= \sum_{i=1}^r \lambda_i \tilde{\mathbf{u}}_i \otimes \tilde{\mathbf{u}}_i \otimes \tilde{\mathbf{u}}_i \end{aligned}$$

where  $\{\tilde{\mathbf{u}}_i\}$  become **orthonormal vectors**

- use the tensor power method to recover  $\{\tilde{\mathbf{u}}_i\}$

# **Tensor completion**

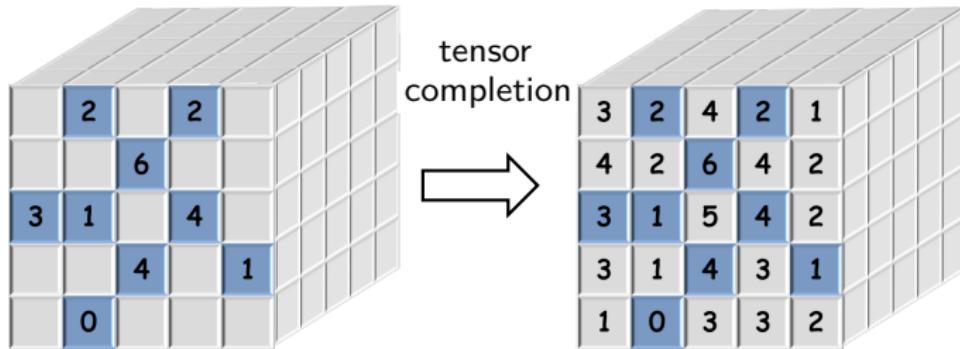
# Another challenge in tensor estimation

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# Tensor completion

**Goal:** faithfully reconstruct unknown tensor from partial observations



Key to enabling reliable reconstruction from incomplete data

— exploiting **low-rank structure**

# Mathematical model

---

- unknown rank- $r$  tensor  $\mathbf{T}^* \in \mathbb{R}^{d \times d \times d}$

$$\mathbf{T}^* = \sum_{i=1}^r \mathbf{u}_i^* \otimes \mathbf{u}_i^* \otimes \mathbf{u}_i^*$$

# Mathematical model

---

- unknown rank- $r$  tensor  $\mathbf{T}^* \in \mathbb{R}^{d \times d \times d}$

$$\mathbf{T}^* = \sum_{i=1}^r \mathbf{u}_i^* \otimes \mathbf{u}_i^* \otimes \mathbf{u}_i^*$$

- partial observations over a random sampling set  $\Omega$

$$T_{i,j,k} = \begin{cases} T_{i,j,k}^*, & (i, j, k) \in \Omega \\ 0, & \text{else} \end{cases}$$

where each location is included in  $\Omega$  independently w.p.  $p$

# Mathematical model

---

- unknown rank- $r$  tensor  $\mathbf{T}^* \in \mathbb{R}^{d \times d \times d}$

$$\mathbf{T}^* = \sum_{i=1}^r \mathbf{u}_i^* \otimes \mathbf{u}_i^* \otimes \mathbf{u}_i^*$$

- partial observations over a random sampling set  $\Omega$

$$T_{i,j,k} = \begin{cases} T_{i,j,k}^*, & (i, j, k) \in \Omega \\ 0, & \text{else} \end{cases}$$

where each location is included in  $\Omega$  independently w.p.  $p$

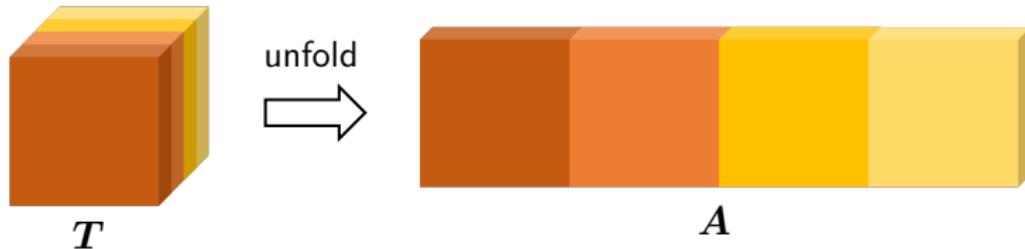
- **goal:** recover  $\mathbf{T}^*$  given  $\mathbf{T}$

# Spectral method (as an initialization scheme)

---

Estimate  $\text{span}\{\mathbf{u}_i^*\}_{1 \leq i \leq r}$

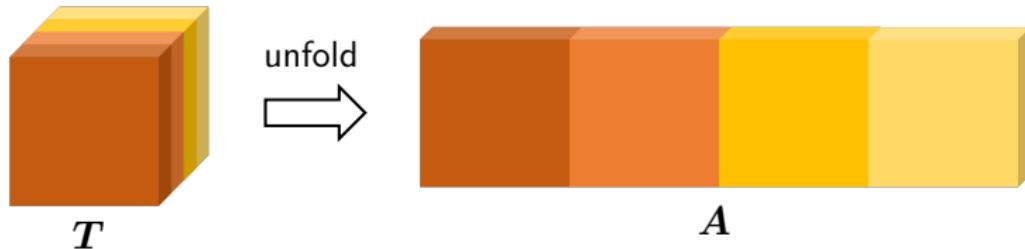
- matricization:  $\mathbf{A} = \text{unfold}(\mathbf{T})$
- estimate rank- $r$  subspace of  $\mathcal{P}_{\text{off-diag}}(\mathbf{A}\mathbf{A}^\top)$  (diagonal deletion)



# Spectral method (as an initialization scheme)

Estimate  $\text{span}\{\mathbf{u}_i^*\}_{1 \leq i \leq r}$

- matricization:  $\mathbf{A} = \text{unfold}(\mathbf{T})$
- estimate rank- $r$  subspace of  $\mathcal{P}_{\text{off-diag}}(\mathbf{A}\mathbf{A}^\top)$  (diagonal deletion)



Iterative refinement via optimization methods (later in this course) ...

# Rationale

---

$$\frac{1}{p^2} \mathbb{E} [\mathbf{A}\mathbf{A}^\top] = \mathbf{A}^* \mathbf{A}^{*\top} + \underbrace{\left( \frac{1}{p} - 1 \right) \mathcal{P}_{\text{diag}}(\mathbf{A}^* \mathbf{A}^{*\top})}_{\text{large bias when } p \text{ is small}}$$

where  $\mathcal{P}_{\text{diag}}$  extracts out diagonal entries

- **issue:** large bias incurred by diagonal entries

# Rationale

---

$$\frac{1}{p^2} \mathbb{E} [\mathbf{A}\mathbf{A}^\top] = \mathbf{A}^* \mathbf{A}^{*\top} + \underbrace{\left( \frac{1}{p} - 1 \right) \mathcal{P}_{\text{diag}}(\mathbf{A}^* \mathbf{A}^{*\top})}_{\text{large bias when } p \text{ is small}}$$

where  $\mathcal{P}_{\text{diag}}$  extracts out diagonal entries

- **issue:** large bias incurred by diagonal entries
- **solution:** suppress diagonal entries, i.e., look at

$$\mathbf{G} = \frac{1}{p^2} \mathcal{P}_{\text{off-diag}}(\mathbf{A}\mathbf{A}^\top)$$

with  $\mathcal{P}_{\text{off-diag}}(\mathbf{M}) := \mathbf{M} - \mathcal{P}_{\text{diag}}(\mathbf{M})$ , which obeys

$$\mathbb{E} [\mathbf{G}] = \mathcal{P}_{\text{off-diag}}(\mathbf{A}^* \mathbf{A}^{*\top}) = \underbrace{\mathcal{P}_{\text{off-diag}}\left(\mathbf{U}^* \boldsymbol{\Sigma}^{*2} \mathbf{U}^{*\top}\right)}_{\text{nearly low-rank under incoherence conditions}}$$

# Theoretical guarantees

## Theorem 5.2 (Informal)

Suppose that the tensor  $T^* \in \mathbb{R}^{d \times d \times d}$  has rank  $r = O(1)$ , and is incoherent and well-conditioned. Then the spectral method returns a consistent estimate of  $\text{span}\{\mathbf{u}_i^*\}_{1 \leq i \leq r}$  as long as

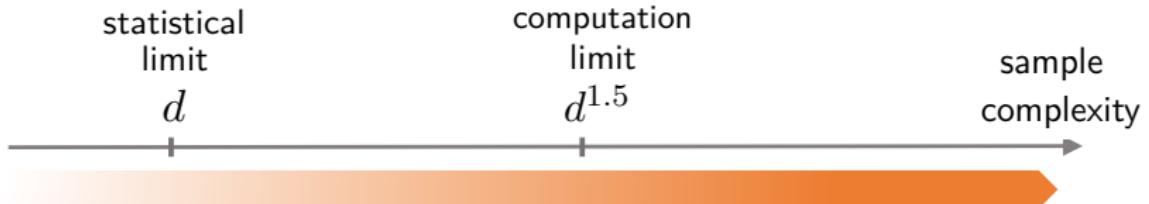
$$p \gtrsim \frac{\text{poly log } d}{d^{1.5}}$$

- see details in Section 3.9 of Chen, Chi, Fan, Ma '21
- consistent estimation is feasible as soon as

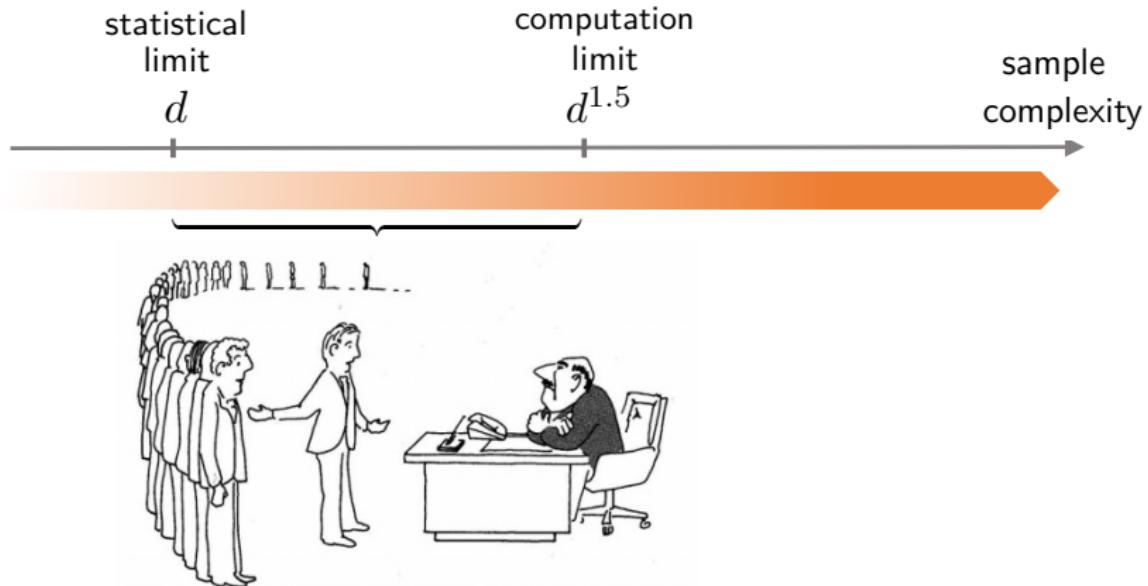
$$\text{sample size } \gtrsim d^{1.5} \text{poly log } d$$

# Statistical-computational gap ( $r = O(1)$ )

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# Statistical-computational gap ( $r = O(1)$ )



*"I can't find an efficient algorithm, but neither can all these people."*

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