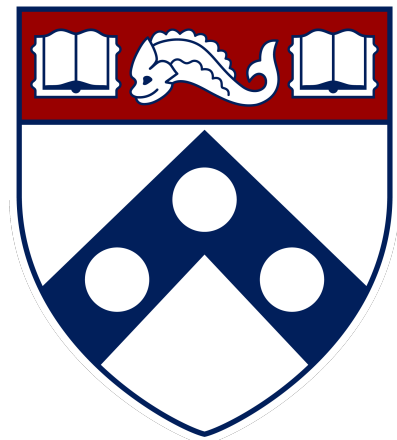
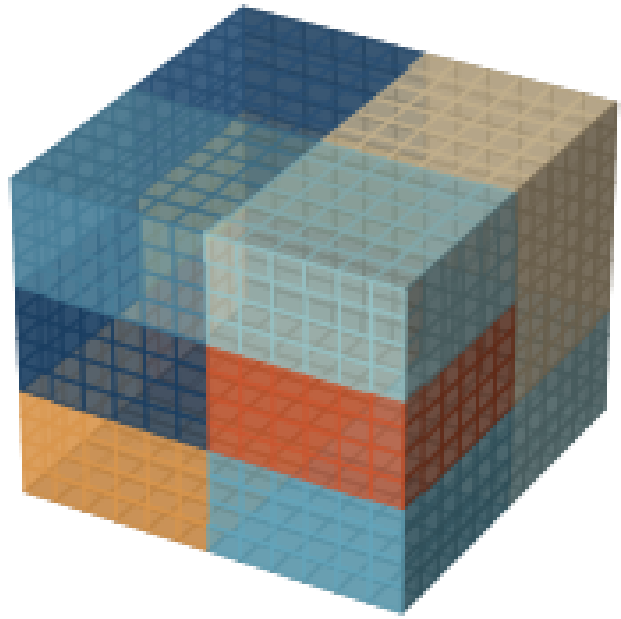
Towards more reliable tensor learning

– heteroskedastic tensor clustering and uncertainty quantification for low-rank tensors



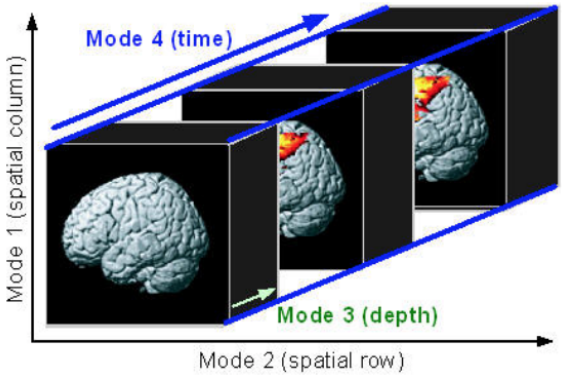
Yuchen Zhou, Wharton Statistics & Data Science

Tensors: high-order arrays



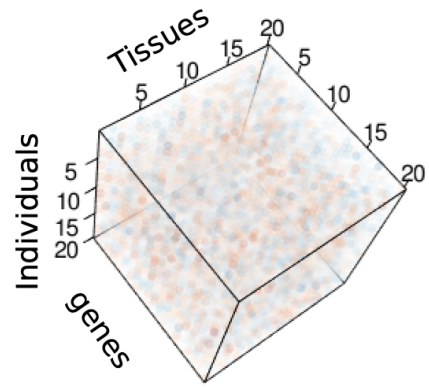
- vectors and matrices are order-1 and order-2 tensors
- $\boldsymbol{\mathcal{X}} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$: order-$d$ tensor

Tensors are everywhere



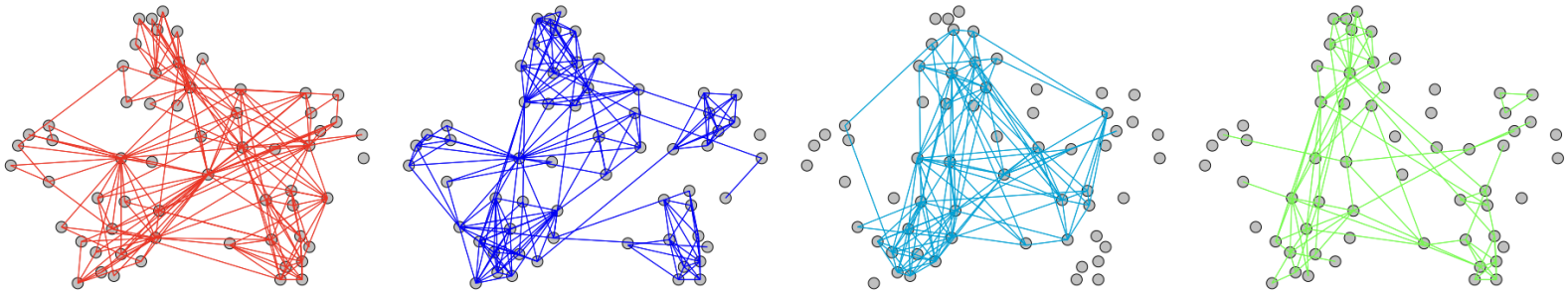
fMRI

fig. credit: Lu et al. '13



Multi-tissue gene expression

fig. credit: Wang et al. '19



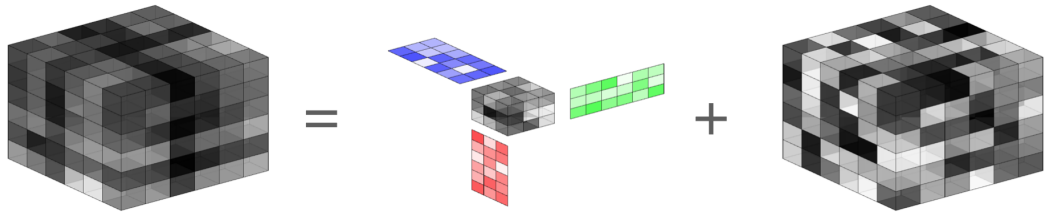
(a) Work. (b) Lunch. (c) Facebook. (d) Friend.

Multilayer network analysis

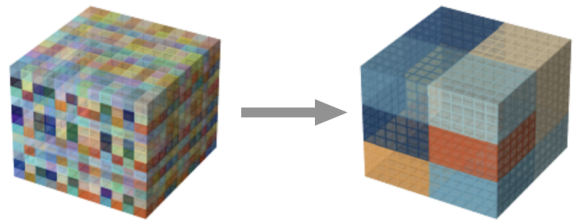
fig. credit: Kim and Lee '15

Various tensor problems

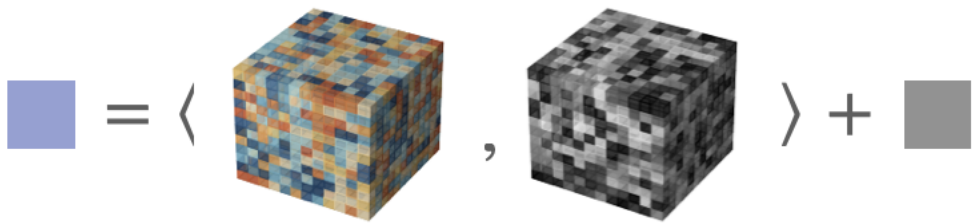
- Tensor SVD/PCA



- Tensor clustering



- Tensor regression



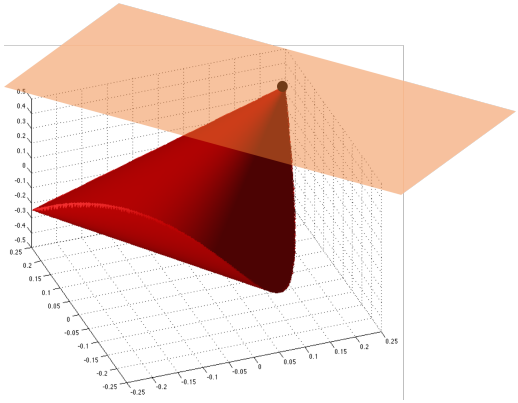
- ...

Foundamental challenges for tensor learning

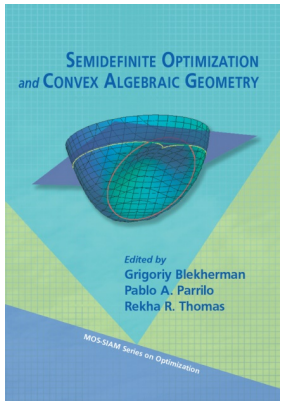
It is NP-hard to compute

- **best low-rank approximation** of tensors
- tensor **spectral norm**
- tensor **nuclear norm**
- ...

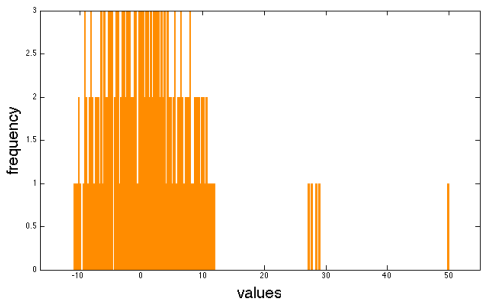
Prior arts



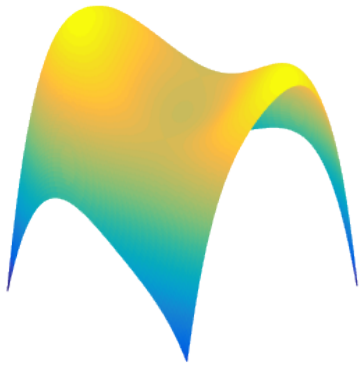
convex relaxation



sum-of-squares



spectral methods



nonconvex optimization

- De Lathauwer et al. '00
- Tomioka and Suzuki '13
- Zhou et al. '13
- Anandkumaret al. '14
- Montanari and Richard '14
- Yuan and Zhang '16
- Rauhut et al. '17
- Sun and Li '17
- Li et al. '18
- Montanari and Sun '18
- Arous et al. '19
- Raskutti et al. '19
- Chi et al. '20
- Zhang et al. '20
- Cai et al. '22
- Han et al. '22
- ...

Prior arts

Challenges remain:

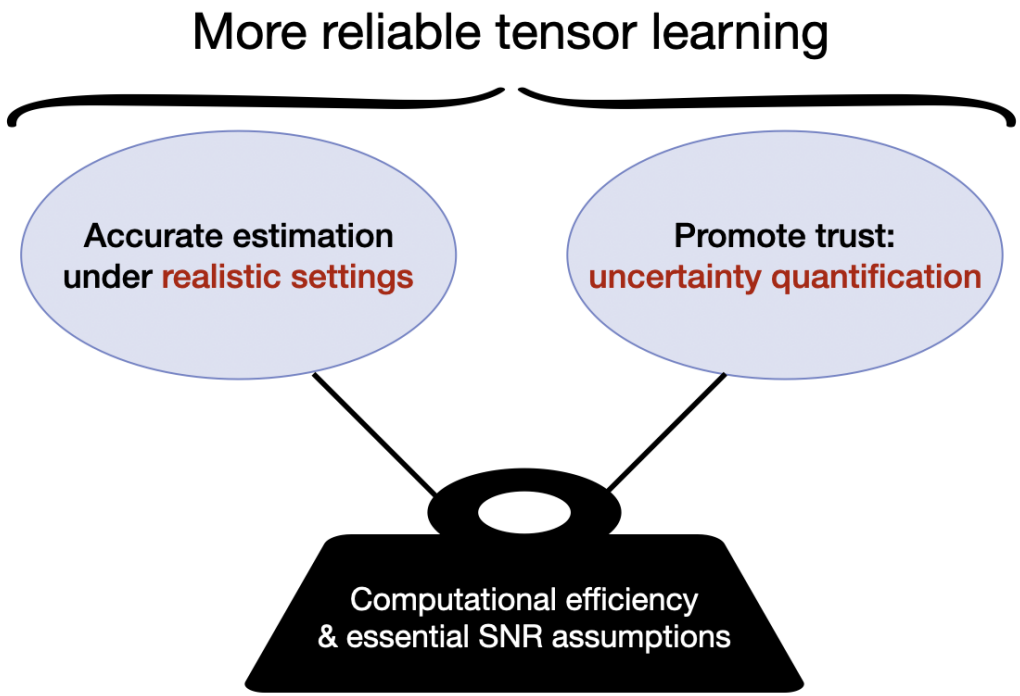
- ideal assumptions (e.g., i.i.d. noise) are often violated
- uncertainty quantification

Prior arts

Challenges remain:

- ideal assumptions (e.g., i.i.d. noise) are often violated
- uncertainty quantification

Can we address these challenges using computationally efficient algorithms? Under essential SNR assumptions?



In this talk...

- **Heteroskedastic** tensor clustering
  - a detour: heteroskedastic PCA

- **Uncertainty quantification** for tensor learning

papers:

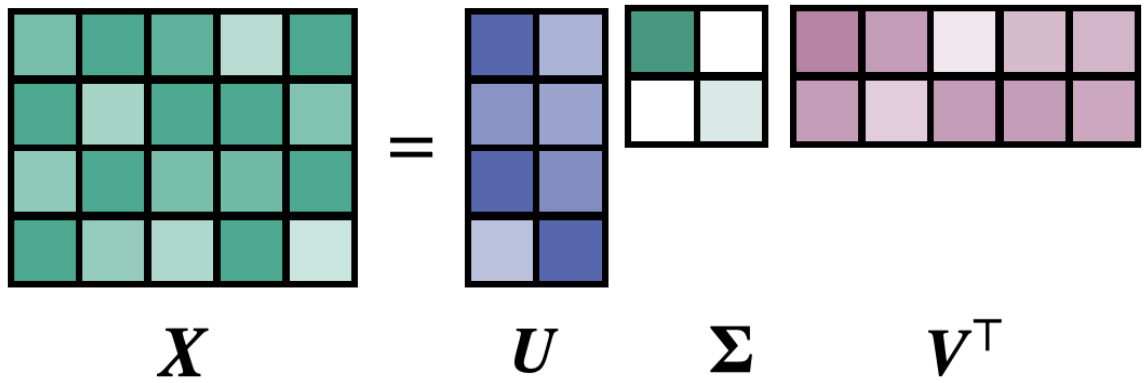
Y. Zhou, Y. Chen, "Deflated HeteroPCA: Overcoming the Curse of Ill-conditioning in Heteroskedastic PCA," under review at *Annals of Statistics*

Y. Zhou, Y. Chen, "Heteroskedastic Tensor Clustering,"under review at *JRSSB*

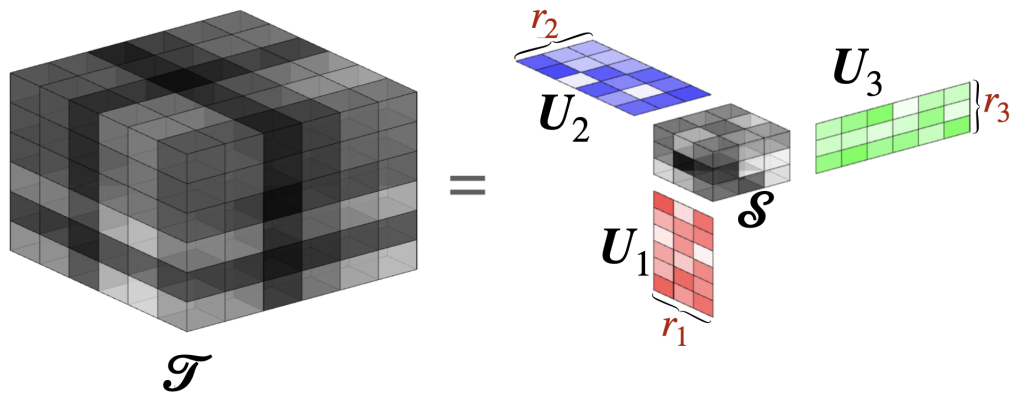
D. Xia, A. Zhang, Y. Zhou, "Inference for Low-rank Tensors – No Need to Debias," *Annals of Statistics*, 2022

Preliminary: Tucker Low-rank Tensors

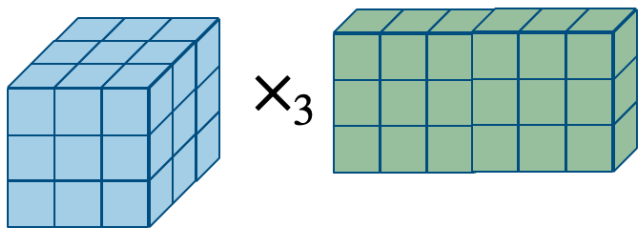
- Matrix SVD



- Tucker decomposition



Preliminary: Tucker Low-rank Tensors



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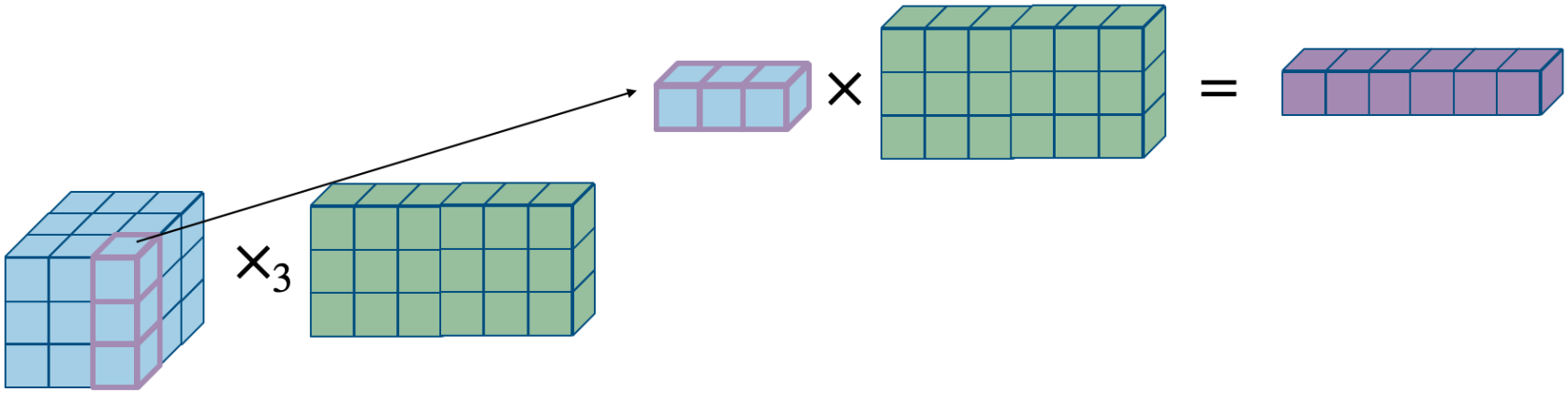

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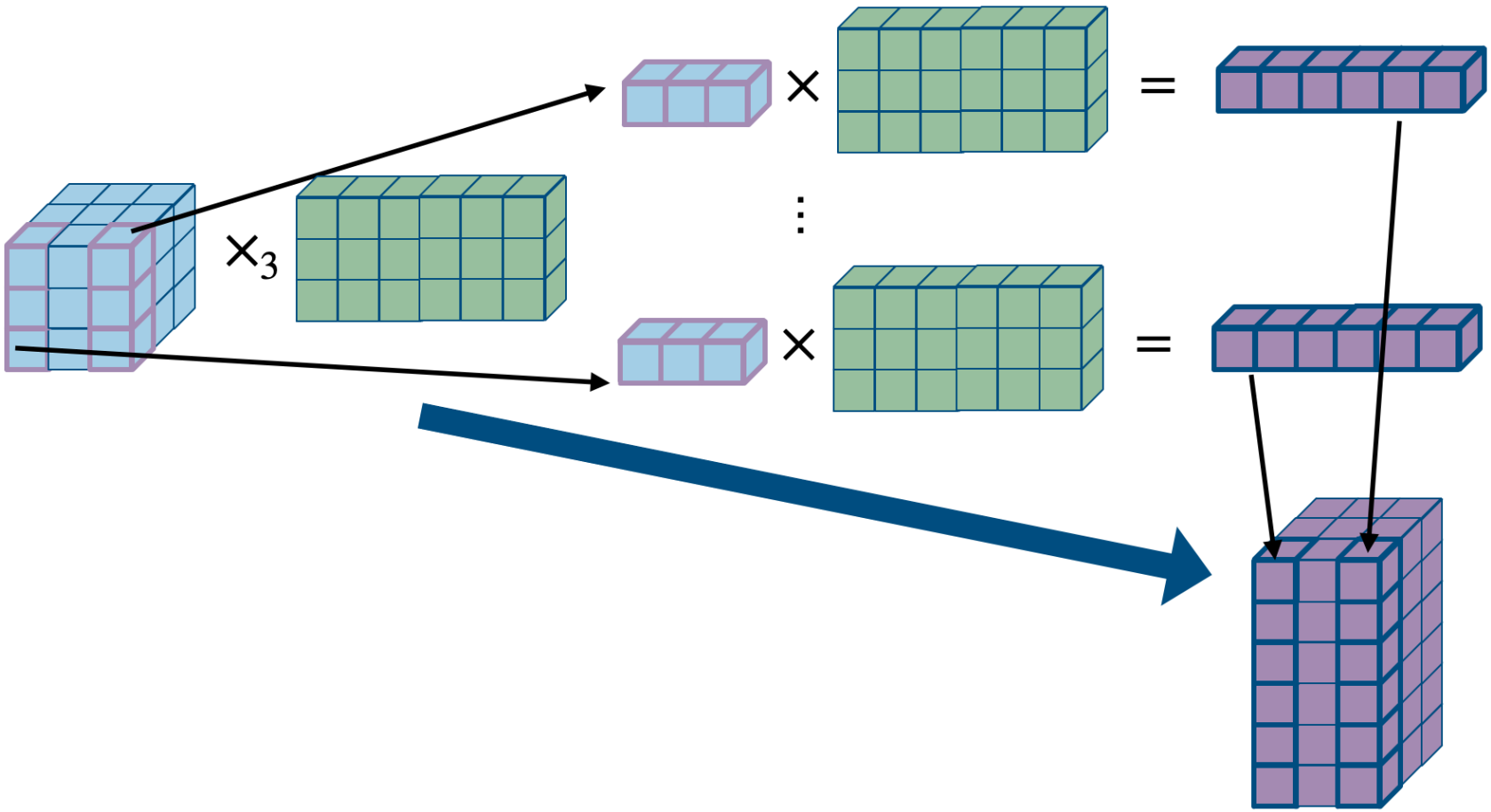

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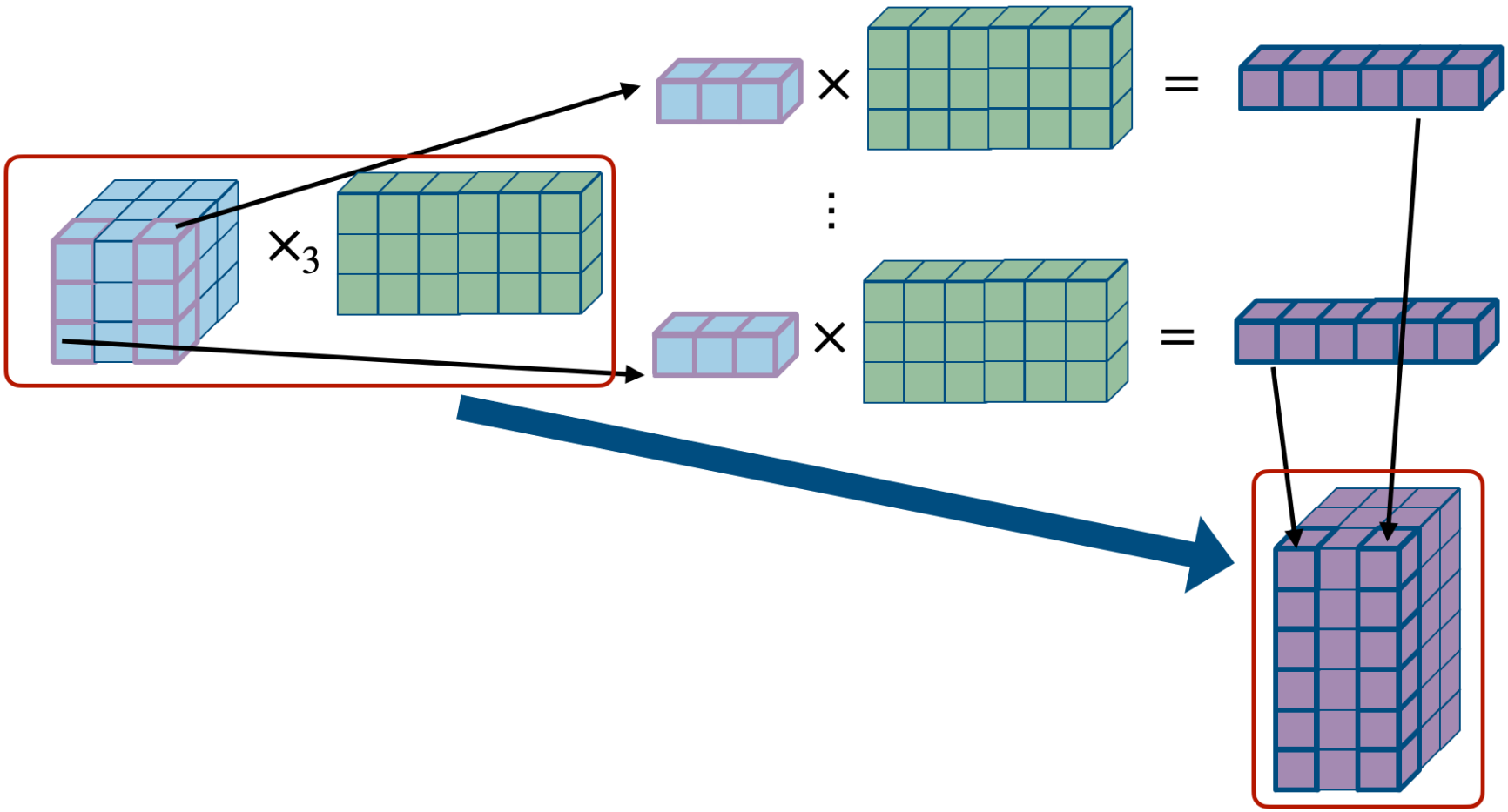
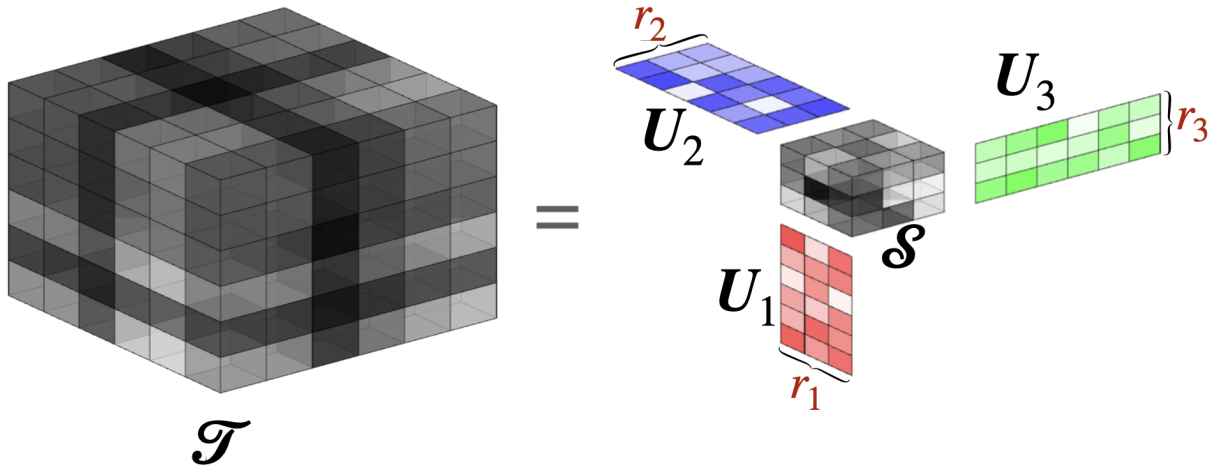


Preliminary: Tucker Low-rank Tensors

$\mathcal{T} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$ has Tucker rank (r_1, r_2, r_3) if

$$\mathcal{T} = \mathcal{S} \times_1 \boldsymbol{U}_1 \times_2 \boldsymbol{U}_2 \times_3 \boldsymbol{U}_3 = (\boldsymbol{U}_1, \boldsymbol{U}_2, \boldsymbol{U}_3) \cdot \mathcal{G},$$

where $\mathcal{S} \in \mathbb{R}^{r_1 \times r_2 \times r_3}$ and $\boldsymbol{U}_i \in \mathbb{O}_{n_i, r_i}$ for $i \in [3]$.



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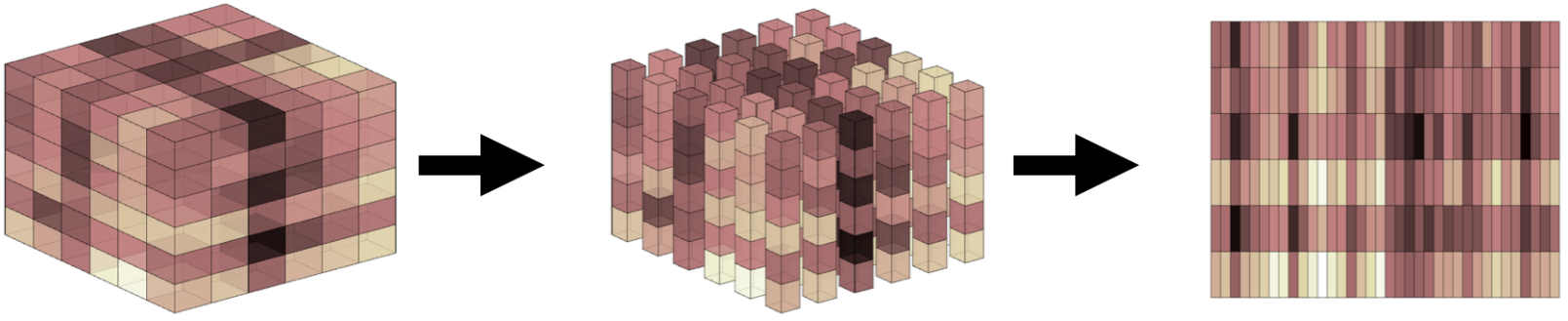
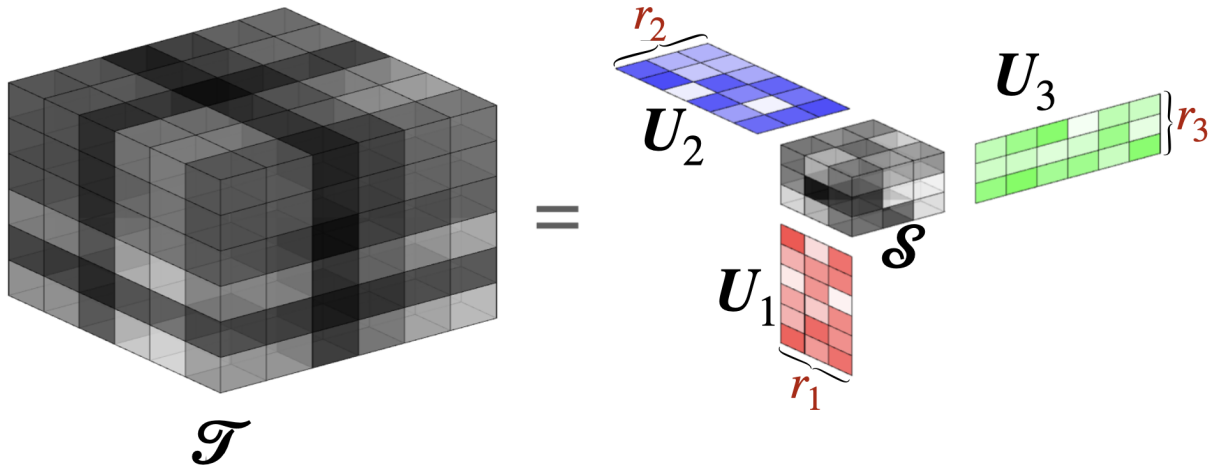


$\mathcal{M}_j(\mathcal{T}) \in \mathbb{R}^{n_j \times (n_1 n_2 n_3 / n_j)}$: jth matricization of $\mathcal{T}$

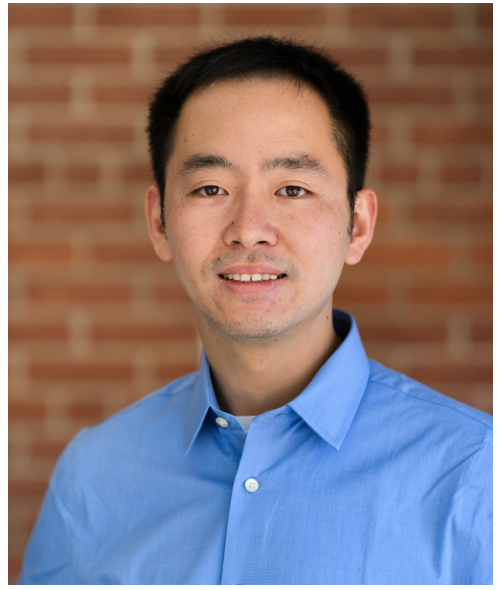
Preliminary: Tucker Low-rank Tensors



$\mathcal{M}_j(\mathcal{T}) \in \mathbb{R}^{n_j \times (n_1 n_2 n_3 / n_j)}$: jth matricization of $\mathcal{T}$

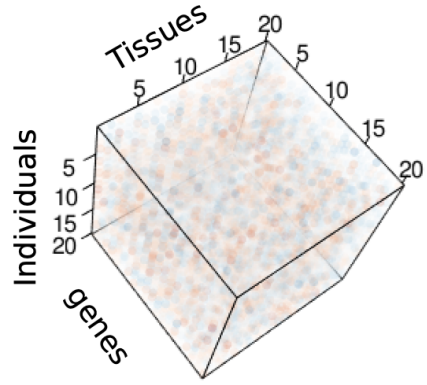
- $\text{rank}(\mathcal{M}_j(\mathcal{T})) = r_j, \quad \forall 1 \leq j \leq 3.$
- U_j is the column subspace of $\mathcal{M}_j(\mathcal{T})$.

Part 1: Heteroskedastic tensor clustering



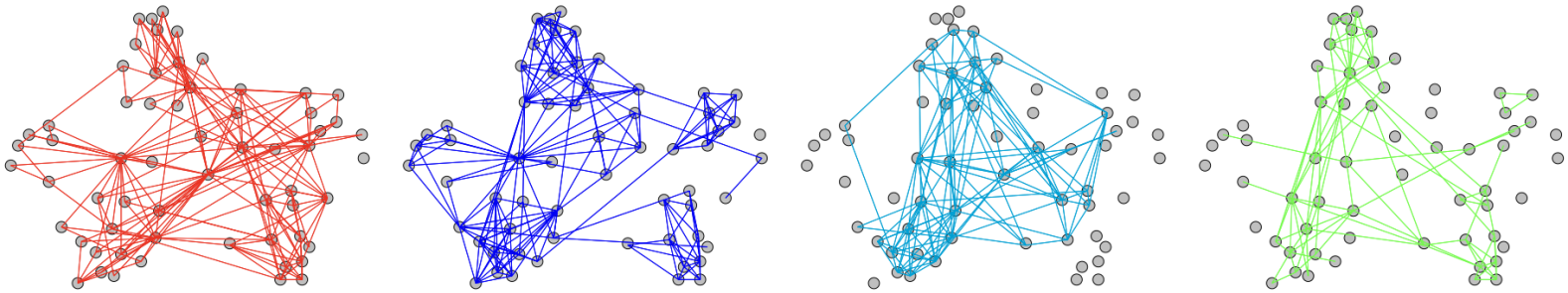
Yuxin Chen
Wharton Statistics & Data Science

Multiway clustering structure



Multi-tissue gene expression

fig. credit: Wang et al. '19

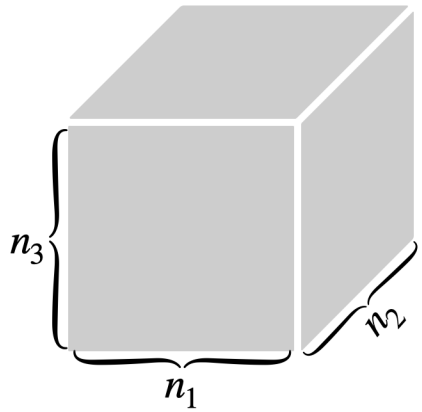


(a) Work. (b) Lunch. (c) Facebook. (d) Friend.

Multilayer network analysis

fig. credit: Kim and Lee '15

Tensor block model



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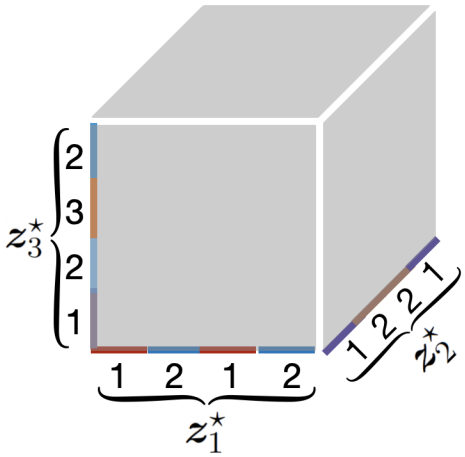
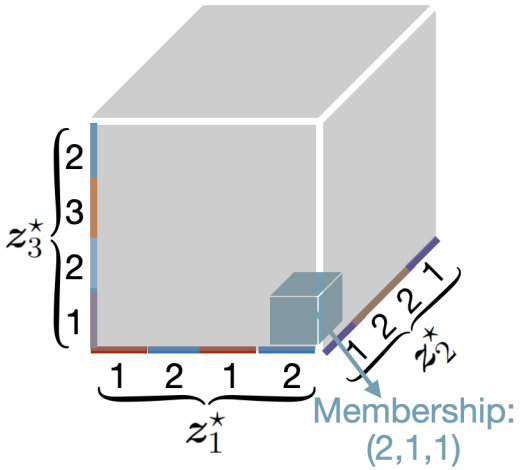


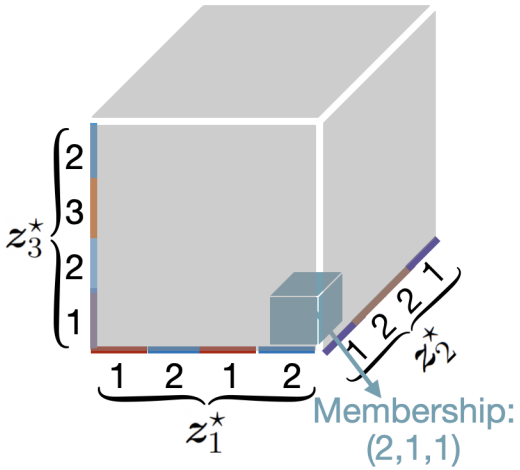
- $\boldsymbol{z}_i^\star \in [k_i]^{n_i}$: cluster assignment vector along the i-th mode
  - $z_{i,j}^\star = \ell$ if the jth index falls within cluster ℓ

Tensor block model



- $\boldsymbol{z}_i^\star \in [k_i]^{n_i}$: cluster assignment vector along the i-th mode
  - $z_{i,j}^\star = \ell$ if the jth index falls within cluster ℓ
  - The membership of (i_1, i_2, i_3) is $(z_{1,i_1}^\star, z_{2,i_2}^\star, z_{3,i_3}^\star)$

Tensor block model



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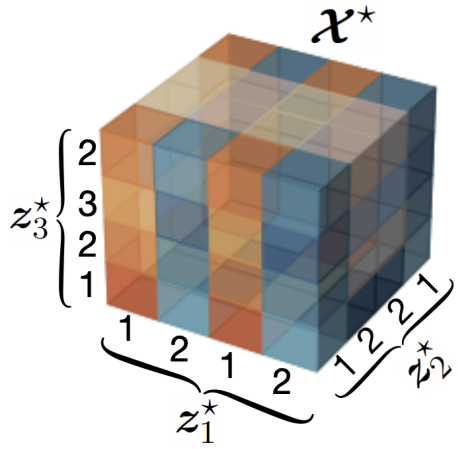
- $\boldsymbol{\mathcal{S}}^\star \in \mathbb{R}^{k_1 \times k_2 \times k_3}$: block/clustering mean

Tensor block model



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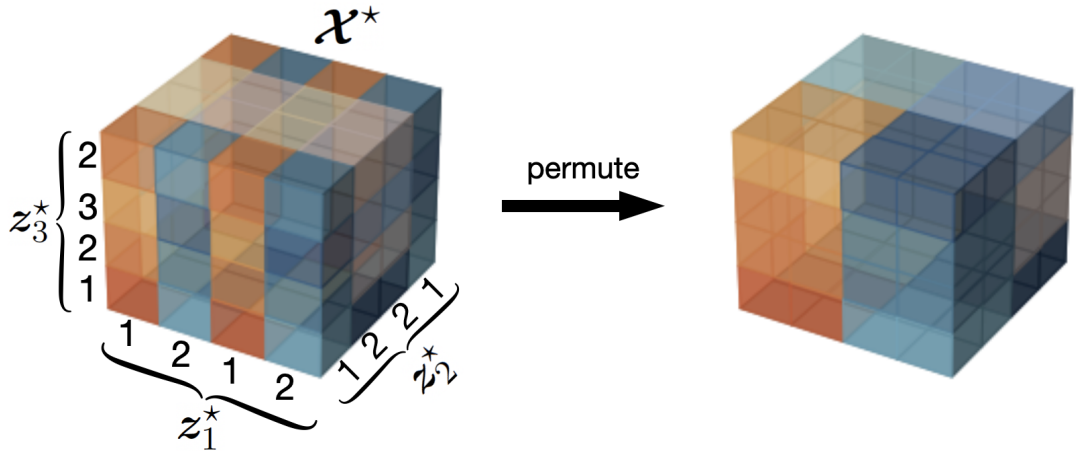
- **Truth:** for all $(i_1, i_2, i_3) \in [n_1] \times [n_2] \times [n_3]$,

$$X^\star_{i_1,i_2,i_3} = S^\star_{z^\star_{1,i_1}, z^\star_{2,i_2}, z^\star_{3,i_3}}.$$

Tensor block model



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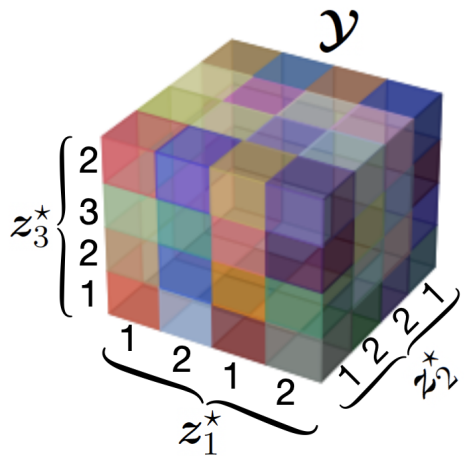
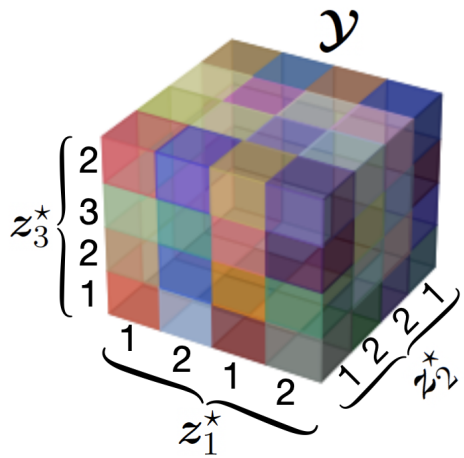
Tensor block model



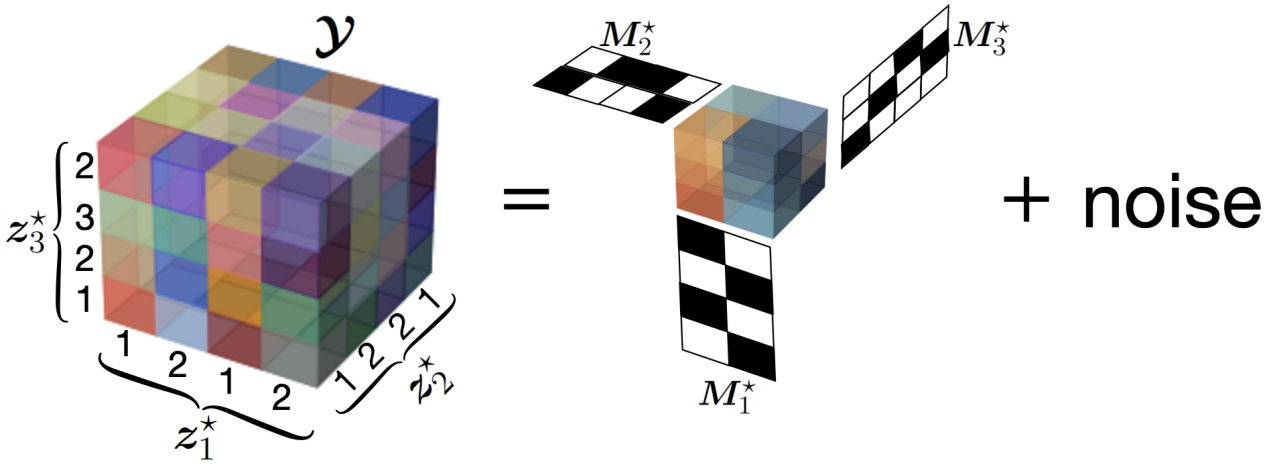
- **Noisy observations:** $\mathcal{Y} = \mathcal{X}^\star + \underbrace{\mathcal{E}}_{\text{zero-mean ind. noise}} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$

Tensor block model



- **Noisy observations:** $\mathcal{Y} = \mathcal{X}^\star + \underbrace{\mathcal{E}}_{\text{zero-mean ind. noise}} \in \mathbb{R}^{n_1 \times n_2 \times n_3}$
- **Goal**: recover $z_i^\star$, $i \in [3]$ from $\mathcal{Y}$

Tensor block model



Equivalently, we observe

$$\mathcal{Y} = \mathcal{X}^\star + \underbrace{\mathcal{E}}_{\text{zero-mean ind. noise}} \in \mathbb{R}^{n_1 \times n_2 \times n_3},$$

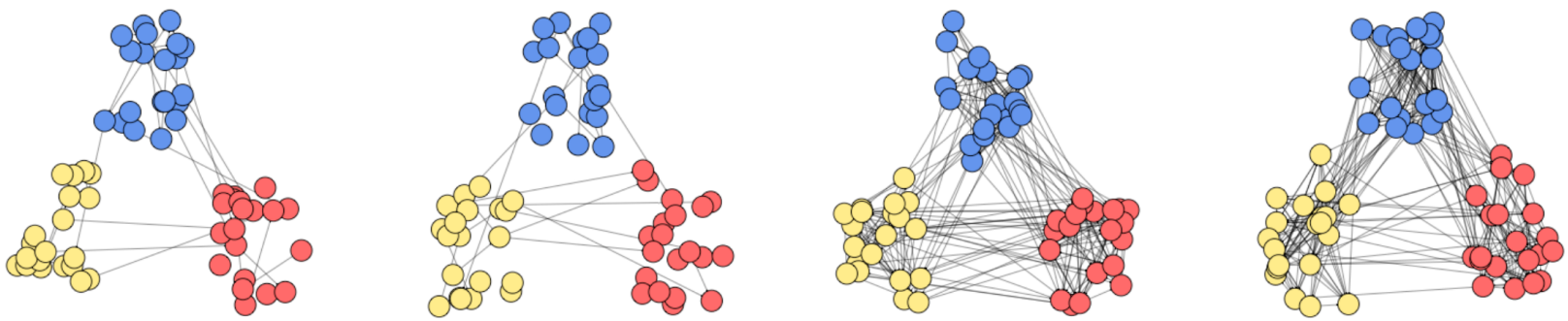
where $\mathcal{X}^\star = \mathcal{S}^\star \times_1 M_1^\star \times_2 M_2^\star \times_3 M_3^\star$, where $M_i^\star \in \{0,1\}^{n_i \times k_i}$ s.t.

$$(M_i^\star)_{j,\ell} = \begin{cases} 1, & \text{if } z_{i,j}^\star = \ell, \\ 0, & \text{else.} \end{cases}$$

An important case: stochastic tensor block model

Stochastic tensor block model (STBM)

- generalization of bipartite stochastic block model
- each entry of $\boldsymbol{\mathcal{S}}^\star$ is connection probability
- $Y_{i,j,\ell} = \begin{cases} 1, & \text{with prob. } S^\star_{z^\star_{1,i}, z^\star_{2,j}, z^\star_{3,\ell}} \\ 0, & \text{o.w.} \end{cases}$ represents if (i, j, ℓ) are connected



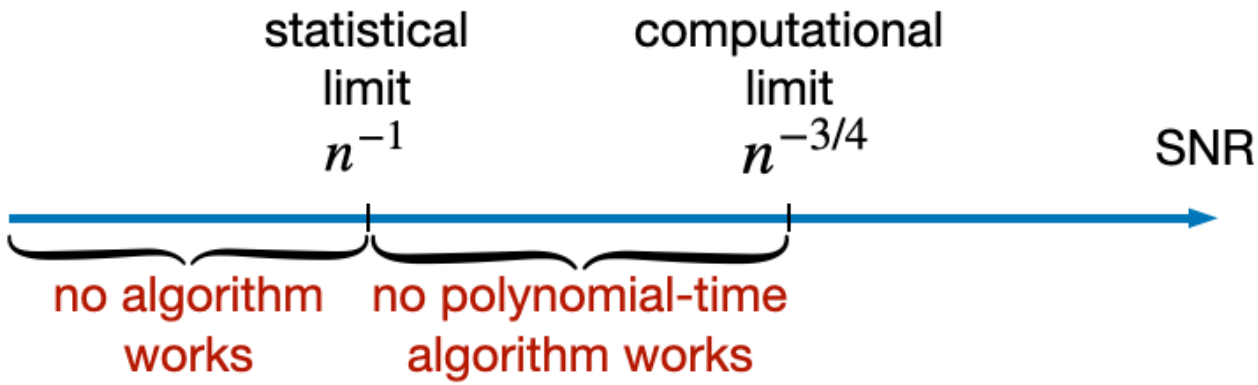
A natural approach

Least-square estimator (Wang and Zeng '19):

$$\left(\widehat{\boldsymbol{\mathcal{S}}}, \widehat{\boldsymbol{z}}_1, \widehat{\boldsymbol{z}}_2, \widehat{\boldsymbol{z}}_3\right) := \underset{\substack{\boldsymbol{\mathcal{S}} \in [k_1]\times[k_2]\times[k_3] \\ \boldsymbol{z}_i \in [k_i]^{n_i}}}{\arg\min} \sum_{i,j,\ell} \left(Y_{i,j,\ell} - S_{z_{1,i}, z_{2,j}, z_{3,\ell}}\right)^2 \qquad (1)$$

- statistically accurate, computationally intractable!

Statistical-computational gap



SNR $:= \Delta_{\min}/\omega_{\max}$, where

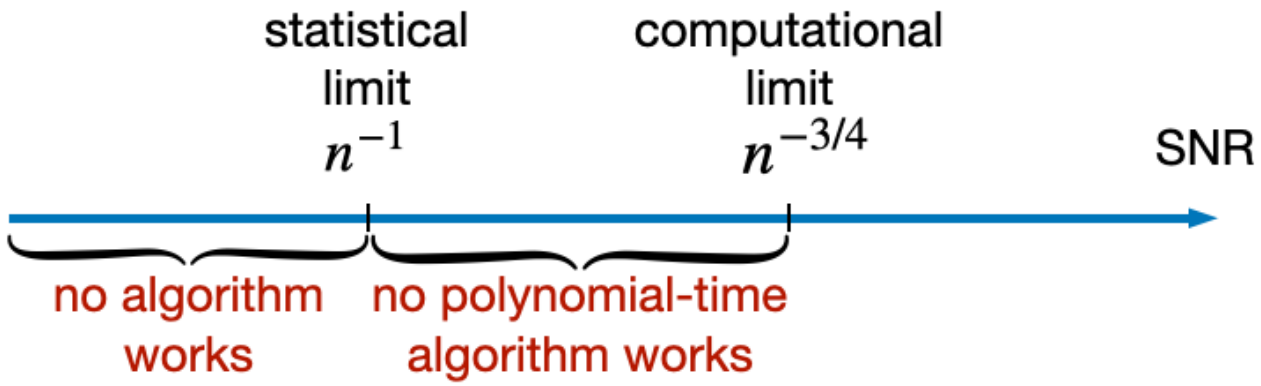
- signal strength:

$$\Delta_1 := \overbrace{\min_{1 \le j_1 \ne j_2 \le k_1} \left\| S^\star_{j_1,:,:} - S^\star_{j_2,:,:} \right\|_2}^{\text{minimum seperation distance along mode}-1}$$

$$\Delta_{\min} := \min_{1 \le i \le 3} \Delta_i$$

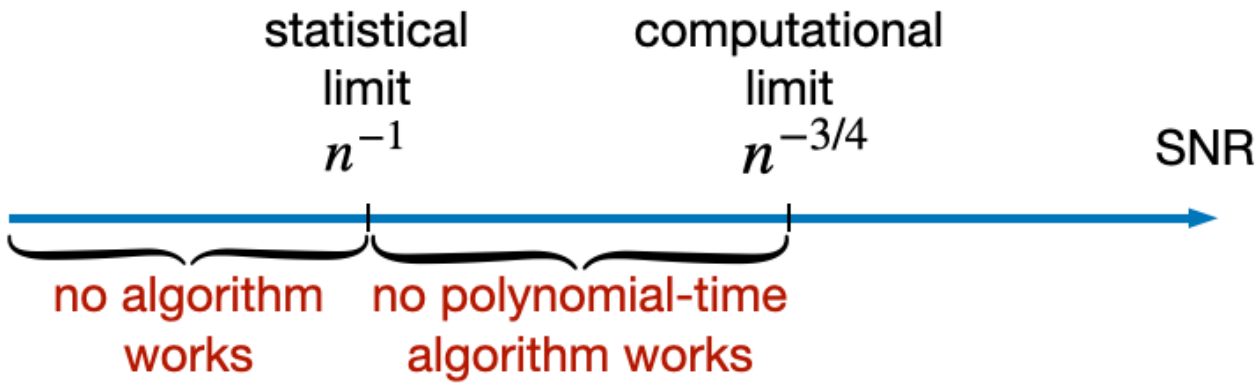
- noise level: $\omega_{\max}$

Statistical-computational gap



- Han et al. '22: HSC + HLloyd
  - spectral clustering + iterative refinements

Statistical-computational gap

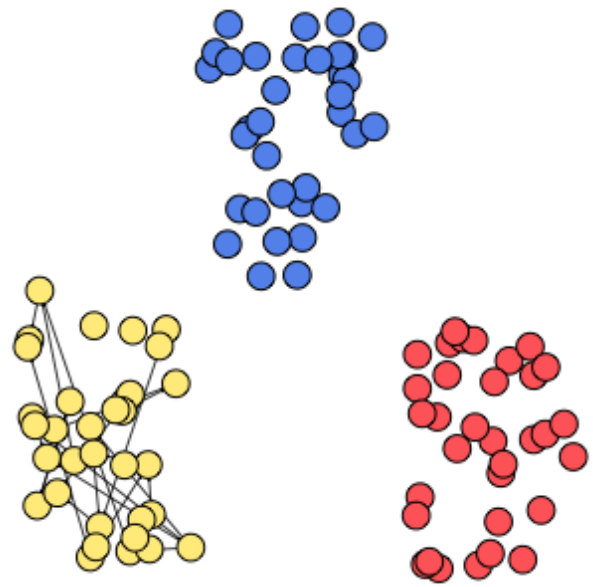


- Han et al. '22: HSC + HLloyd
  - spectral clustering + iterative refinements

- Under i.i.d. sub-Gaussian noise, HSC + HLloyd achieves exact clustering if SNR exceeds $n^{-3/4}$ (up to log factors)

A toy example: STBM

- 100-layer networks, with 100 nodes
- 3 clusters for layers, 3 clusters for nodes
- Nodes within the yellow/red/blue community are sparsely connected.



Layer 1

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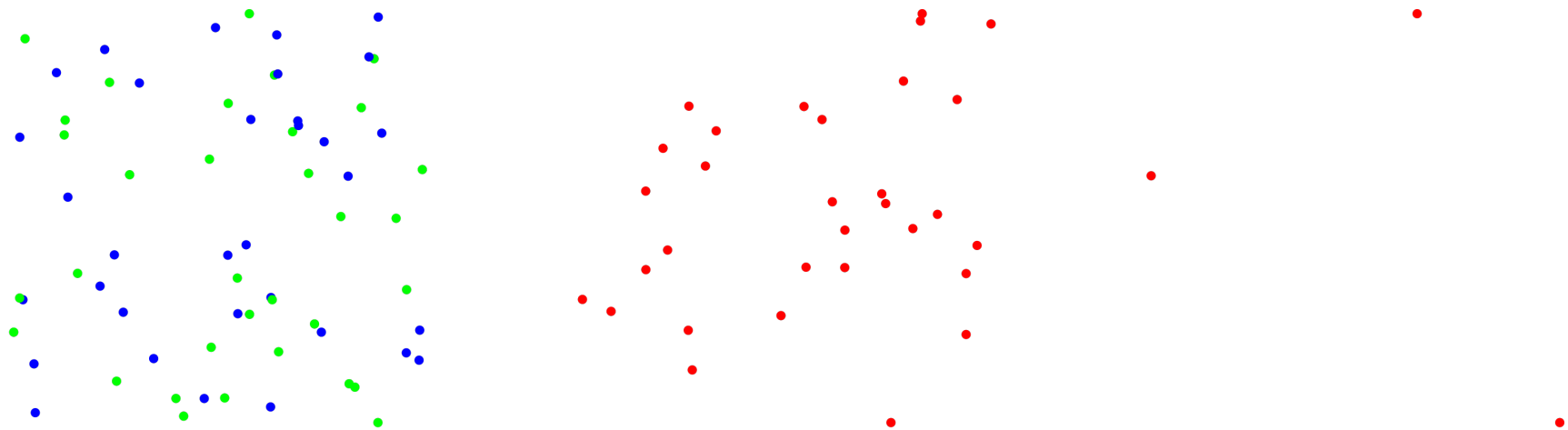

HSC

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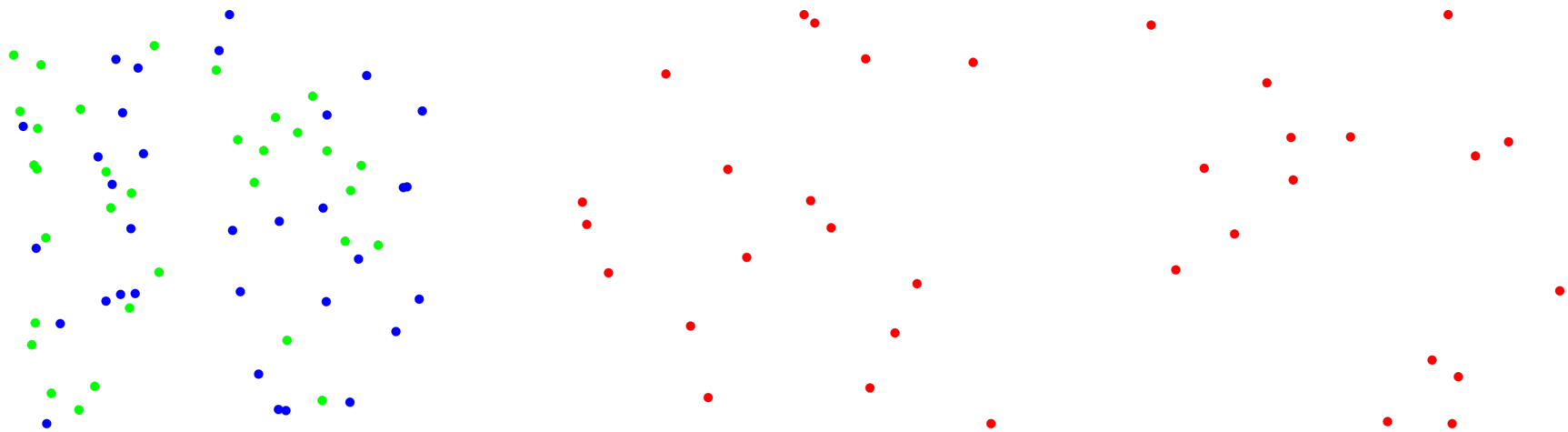


HSC + HLloyd

A common senario: heteroskedastic noise

- noise variances $\underbrace{\{\mathbb{E}[E_{i,j,\ell}^2]\}}_{\text{unknown } \textit{a priori}}$ are location-varying

- discrete-valued observations: multi-tissue gene expression data, multilayer network data

A common senario: heteroskedastic noise

- noise variances $\underbrace{\{\mathbb{E}[E_{i,j,\ell}^2]\}}_{\text{unknown } \textit{a priori}}$ are location-varying
- discrete-valued observations: multi-tissue gene expression data, multilayer network data
- fail dramatically in the face of **heteroskedastic** noise!

How to deal with heteroskedastic noise under essential SNR conditions?

Spectral clustering

- Step 1: estimate "important" subspaces of $\boldsymbol{X}_i^\star = \mathcal{M}_i(\boldsymbol{\mathcal{X}}^\star)$

- Step 2: apply approximate k-means on the rows of

$$\widehat{\boldsymbol{B}}_i = \mathcal{M}_i(\boldsymbol{\mathcal{Y}} \underbrace{\times_i \boldsymbol{U}_i \boldsymbol{U}_i^\top}_{\text{denoising}} \underbrace{\times_{i+1} \boldsymbol{U}_{i+1} \times_{i+2} \boldsymbol{U}_{i+2}}_{\text{dimension reduction \& denoising}})$$

  - can be efficiently done by using k-means++!

Spectral clustering

- Step 1: estimate "important" subspaces of $\boldsymbol{X}_i^\star = \mathcal{M}_i(\boldsymbol{\mathcal{X}}^\star)$

Key challenges:

- unbalanced dimensionality
- heteroskedastic noise

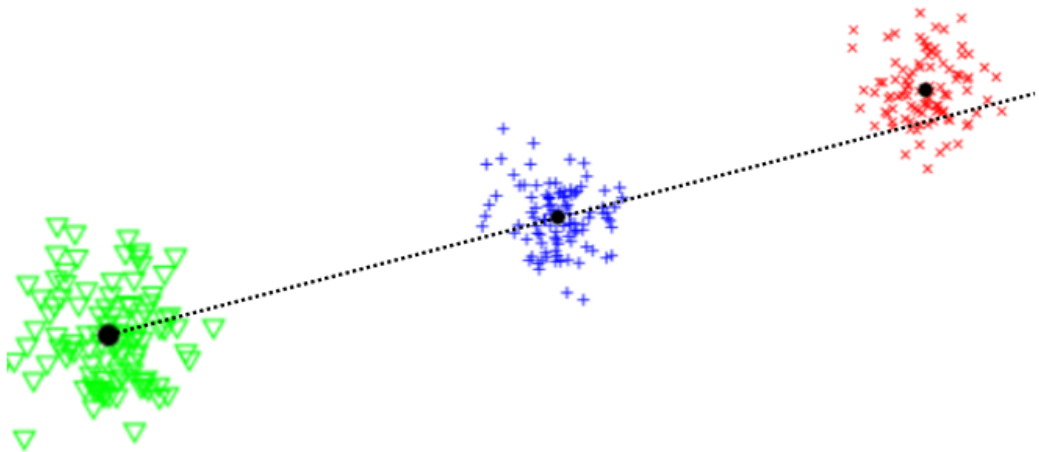
SVD can be highly sub-optimal $\Longrightarrow$ HSC fails drastically!

Spectral clustering

- Step 1: estimate "important" subspaces of $\boldsymbol{X}_i^\star = \mathcal{M}_i(\boldsymbol{\mathcal{X}}^\star)$

Key challenges:

- avoid unnecessary assumptions on condition number of $\boldsymbol{\mathcal{S}}^\star$



condi. number $\kappa := \frac{\max_i \sigma_1(\mathcal{M}_i(\boldsymbol{\mathcal{S}}^\star))}{\min_i \sigma_{k_i}(\mathcal{M}_i(\boldsymbol{\mathcal{S}}^\star))}$

Road map

Subspace estimation problem

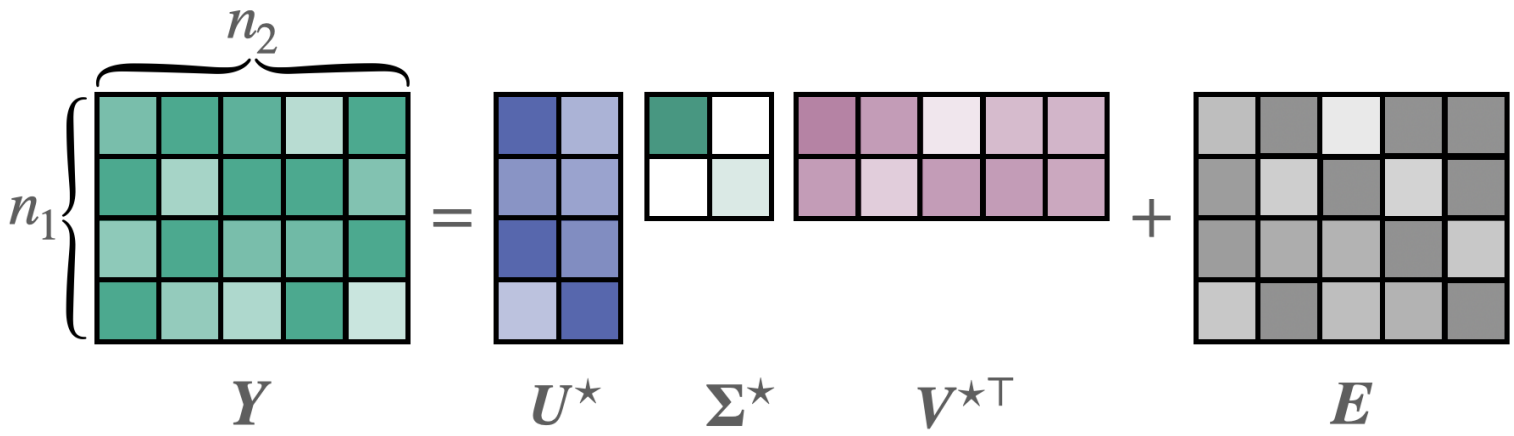
- Key challenges: heteroskedastic noise
  unbalanced dimensionality
  not well-conditioning
- Propose Deflated HeteroPCA! 

More reliable solution to PCA problem!

Spectral tensor clustering

- Still need assumptions on least singular value
- Thresholded Deflated HeteroPCA + k-means!

A detour: a subspace estimation / model



- **Ground truth:** rank-r matrix $\boldsymbol{X}^\star$ with SVD ($r \ll \min\{n_1, n_2\}$)

$$\boldsymbol{X}^\star = \boldsymbol{U}^\star \boldsymbol{\Sigma}^\star \boldsymbol{V}^{\star\top} = \sum_{i=1}^{r} \sigma_i^\star \boldsymbol{u}_i^\star \boldsymbol{v}_i^{\star\top} \in \mathbb{R}^{n_1 \times n_2}$$

where $\boldsymbol{U}^\star \in \mathbb{R}^{n_1 \times r}$, $\boldsymbol{\Sigma}^\star = \mathsf{diag}\{\sigma_1^\star, \cdots, \sigma_r^\star\}$, $\boldsymbol{V}^\star \in \mathbb{R}^{n_2 \times r}$

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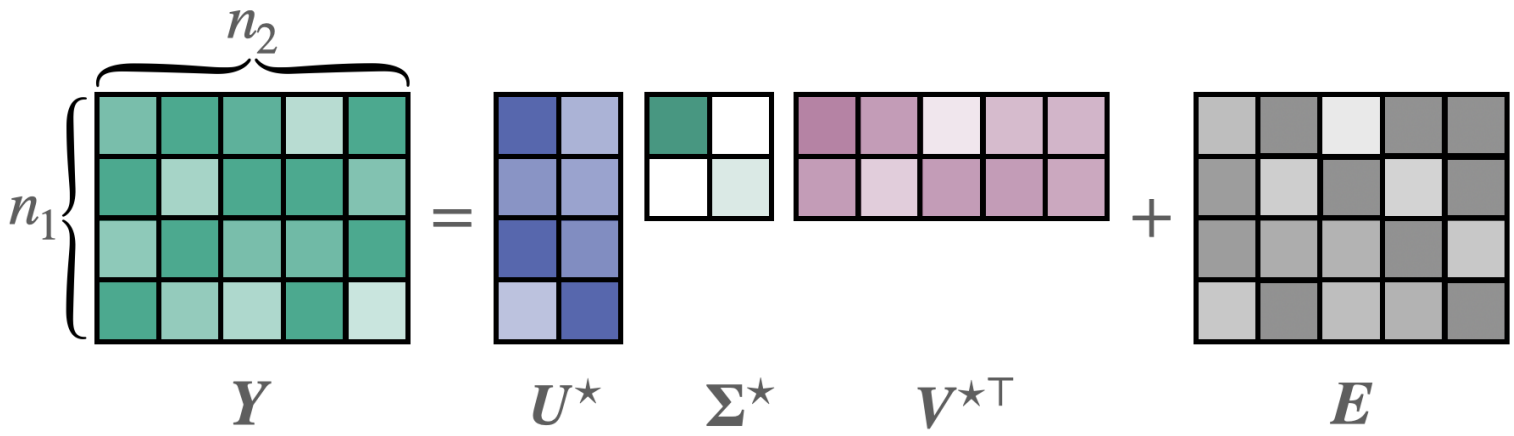

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zero-mean ind. noise

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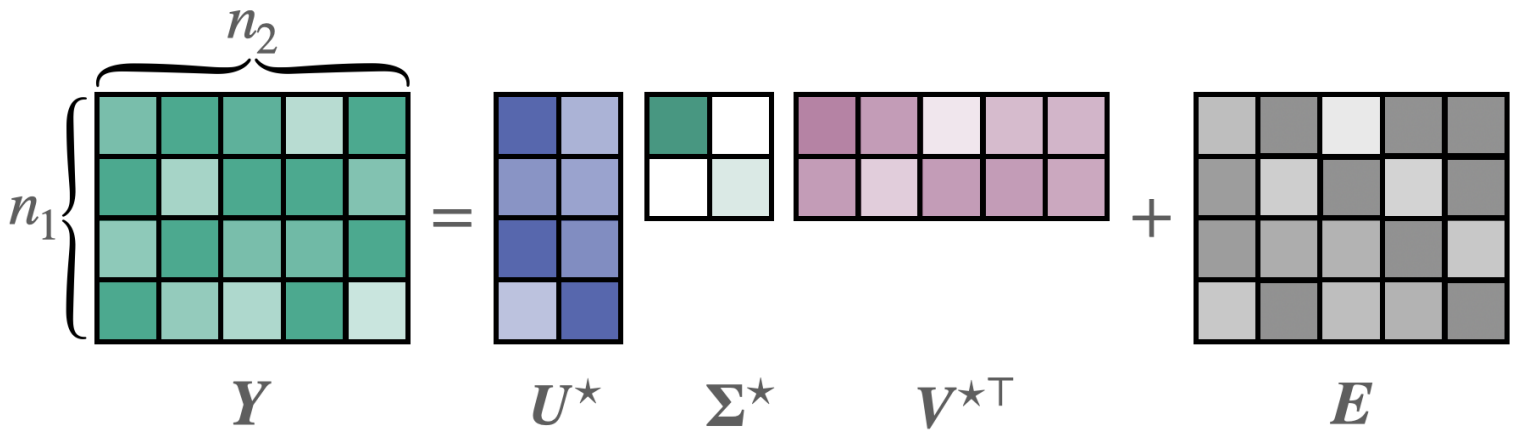

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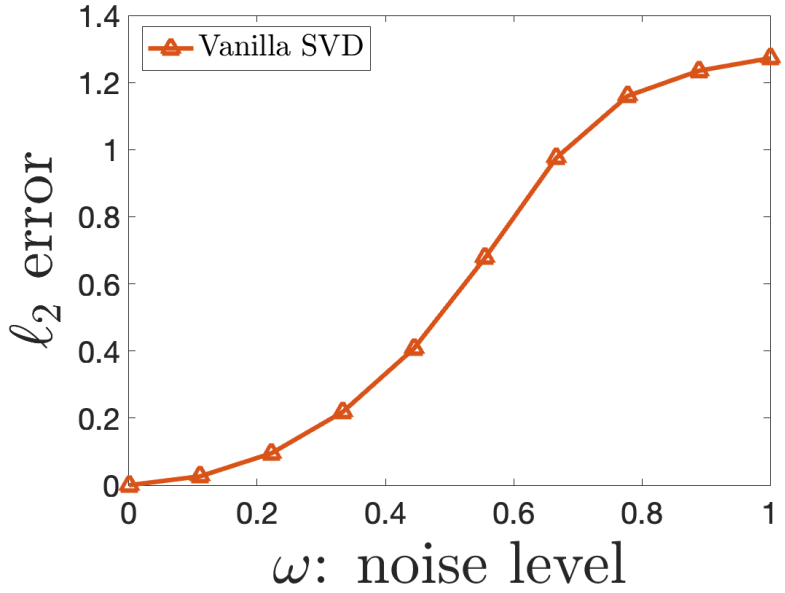
- **Noisy observations:** $\boldsymbol{Y} = \boldsymbol{X}^\star + \underbrace{\boldsymbol{E}}_{\text{zero-mean ind. noise}}$
- **Goal**: estimate column subspace $\boldsymbol{U}^\star \in \mathbb{R}^{n_1 \times r}$ based on $\boldsymbol{Y}$

Review of popular methods

$$n_1 = 100, n_2 = 10,000$$

$$r = 2, \kappa := \sigma_1^\star / \sigma_r^\star = 2$$

$$\omega_i \overset{\text{ind.}}{\sim} \mathsf{Unif}([0, \omega]),\ E_{i,j} \overset{\text{ind.}}{\sim} \mathcal{N}(0, \omega_i^2)$$



vanilla SVD: $U \longleftarrow$ rank-r left singular subspace of $\boldsymbol{Y} = \boldsymbol{X}^\star + \boldsymbol{E}$

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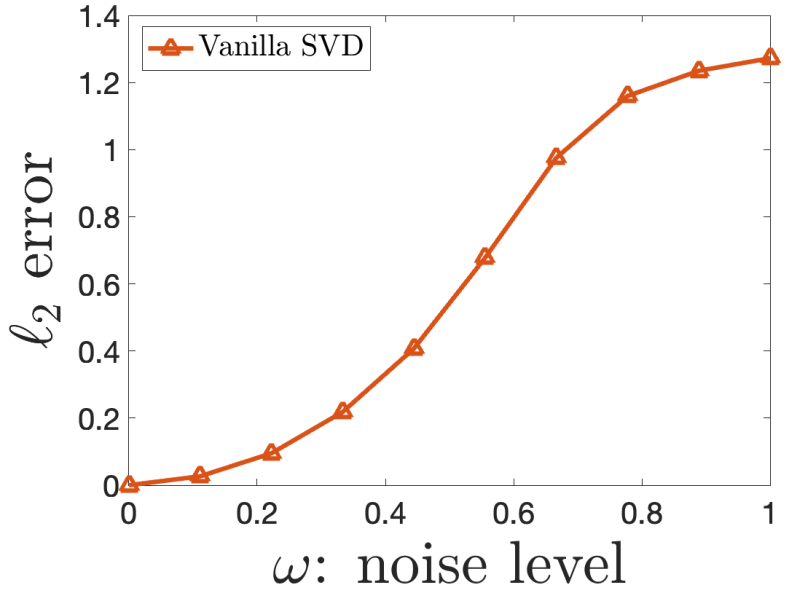

vanilla SVD: $U \longleftarrow$ rank-r left singular subspace of $\boldsymbol{Y} = \boldsymbol{X}^\star + \boldsymbol{E}$

- often sub-optimal due to large bias in diagonal entries:

$$\mathbb{E}\left[\boldsymbol{Y}\boldsymbol{Y}^\top\right] = \underbrace{\boldsymbol{X}^\star\boldsymbol{X}^{\star\top}}_{\checkmark} + \underbrace{\mathsf{diag}\left\{\left[\sum\nolimits_j \mathbb{E}[E_{i,j}^{\star 2}]\right]_{1\le i\le n_1}\right\}}_{\text{potentially large diagonal matrix!}}$$

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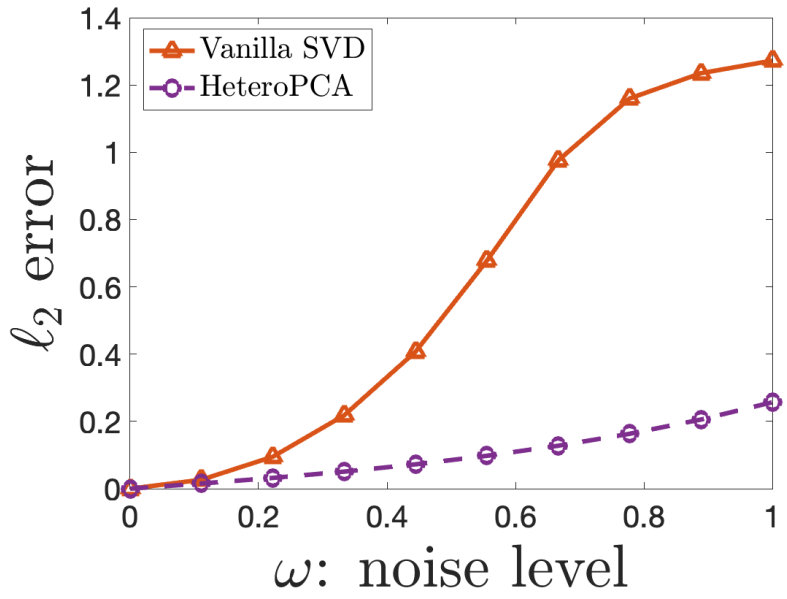

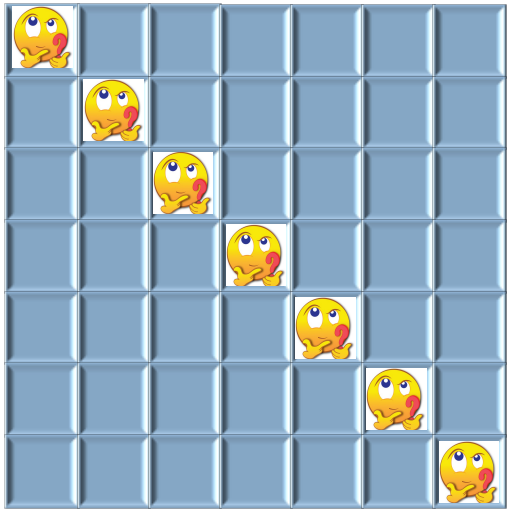

HeteroPCA (Zhang, Cai, Wu '22)

- remove diag($\boldsymbol{Y}\boldsymbol{Y}^\top$) & compute top-$r$ eigen-space
- iteratively estimate diag($\boldsymbol{X}\boldsymbol{X}^\top$)
- compute top-r eigen-space

Review of popular methods

$$n_1 = 100, n_2 = 10,000$$

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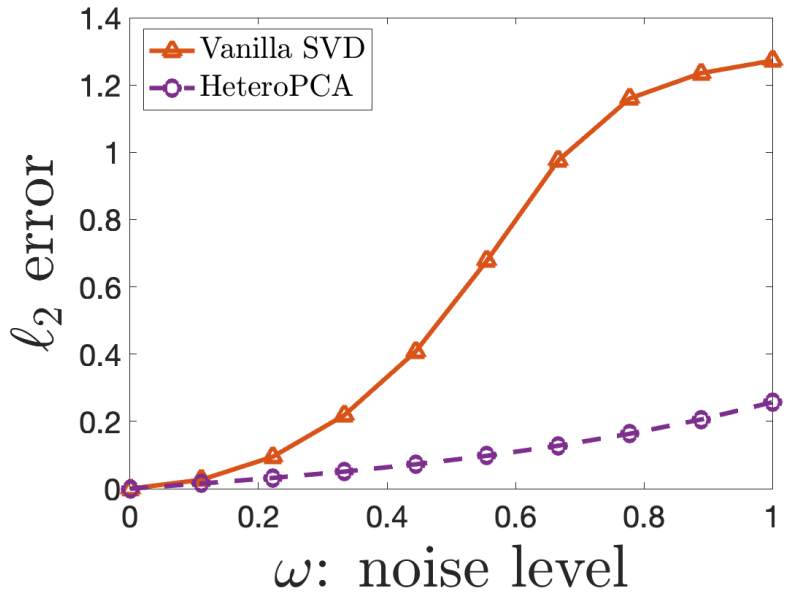
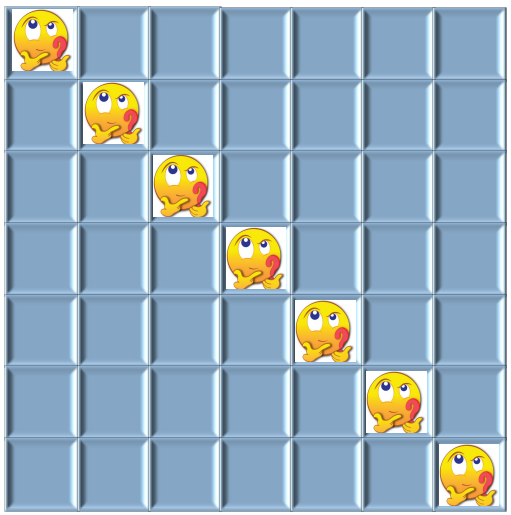




HeteroPCA (Zhang, Cai, Wu '22)

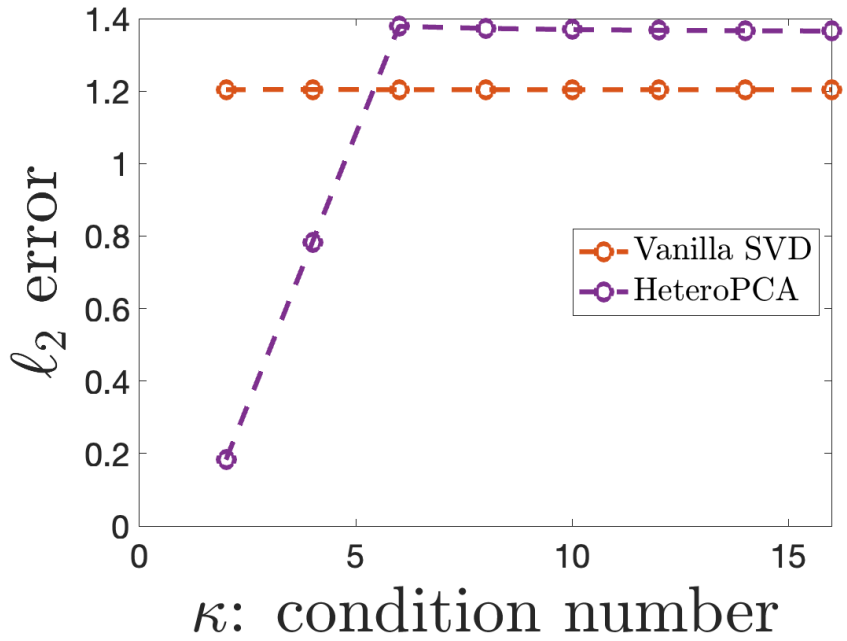
- **initialize:** $\boldsymbol{G}^0 = \mathcal{P}_{\text{off-diag}}(\boldsymbol{Y}\boldsymbol{Y}^\top)$
- for $t = 0, 1, \ldots$

$$(\boldsymbol{U}^t, \boldsymbol{\Lambda}^t) = \mathsf{eigs}(\boldsymbol{G}^t, r)$$

$$\boldsymbol{G}^{t+1} = \boldsymbol{G}^0 + \mathcal{P}_{\mathsf{diag}}(\boldsymbol{U}^t \boldsymbol{\Lambda}^t \boldsymbol{U}^{t\top})$$

A curious phenomenon: curse of ill-conditioning

Somewhat surprising numerical example: $r = 2, n_1 = 200,\ n_2 = 40,000$



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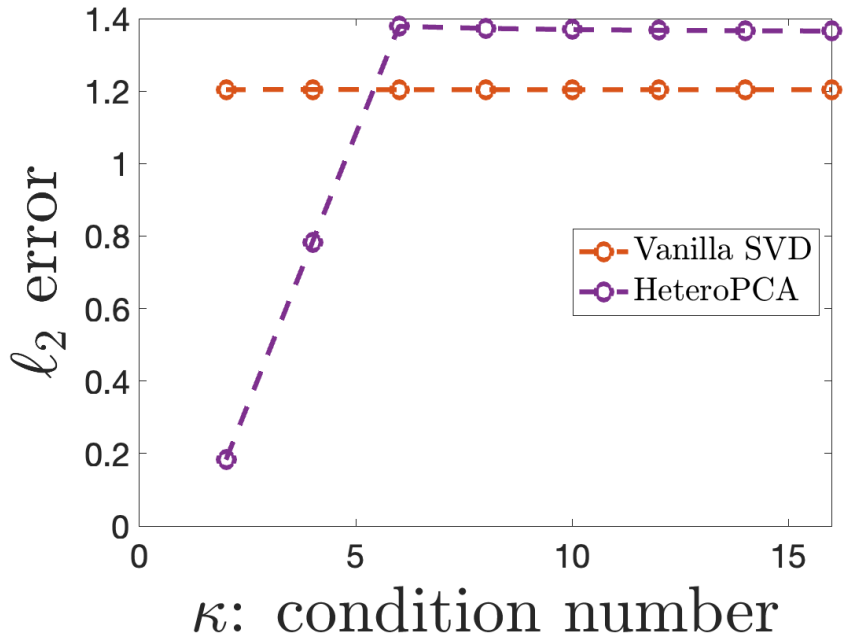
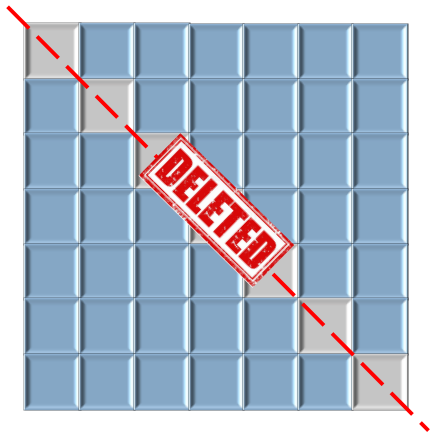


Previous methods degrade as *condition number of $\boldsymbol{X}^\star$ increases*!

but this actually makes problem info-theoretically easier ...

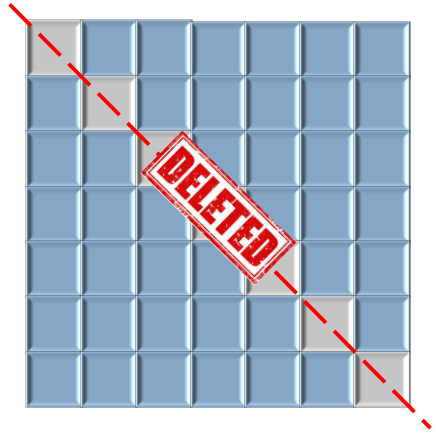
Diagonsis: influences of diagonal deletion



$$\mathbb{E}\Big[\mathcal{P}_{\text{off-diag}}\big(\boldsymbol{Y}\boldsymbol{Y}^\top\big)\Big] = \boldsymbol{X}^\star\boldsymbol{X}^{\star\top} - \underbrace{\mathcal{P}_{\text{diag}}\big(\boldsymbol{X}^\star\boldsymbol{X}^{\star\top}\big)}_{\text{ideally negligible compared to } \sigma_r^{\star 2}}$$

- ideally, we hope diagonal deletion has negligible influences

Diagonsis: influences of diagonal deletion



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but larger than $\sigma_r^{\star 2}$ if $\sigma_1^\star/\sigma_r^\star$ is too large

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- non-negligible for ill-conditioned case though ...

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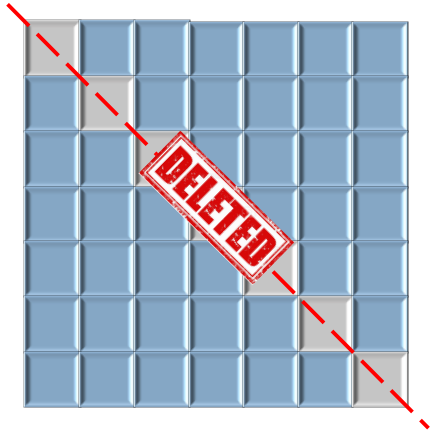

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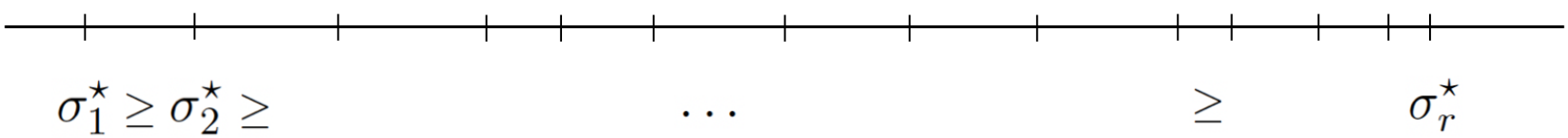
HeteroPCA becomes ineffective in the presence of ill-conditioning!

Can we break the curse of ill-conditioning while accommodating widest SNR range?

— *Zhang et al. '18, Yan et al. '21*

revisit HeteroPCA theory: works well if

- $\boldsymbol{X}^\star$ is well-conditioned
- least singular value $\sigma_r^\star$ (or spectral gap) is not buried by noise



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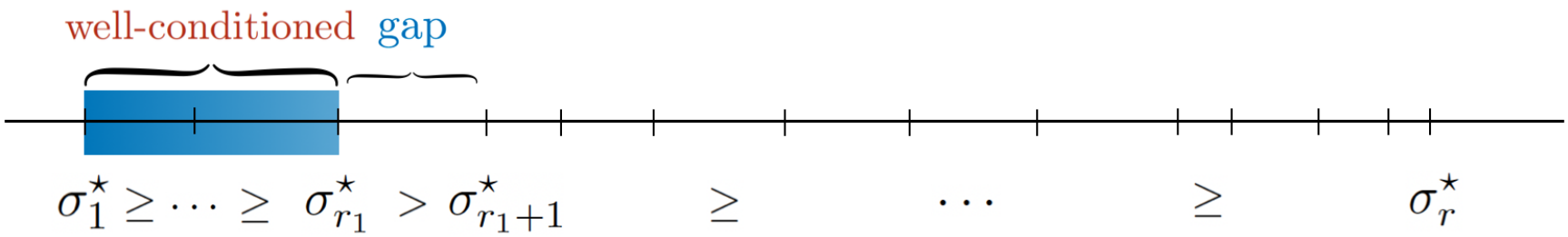
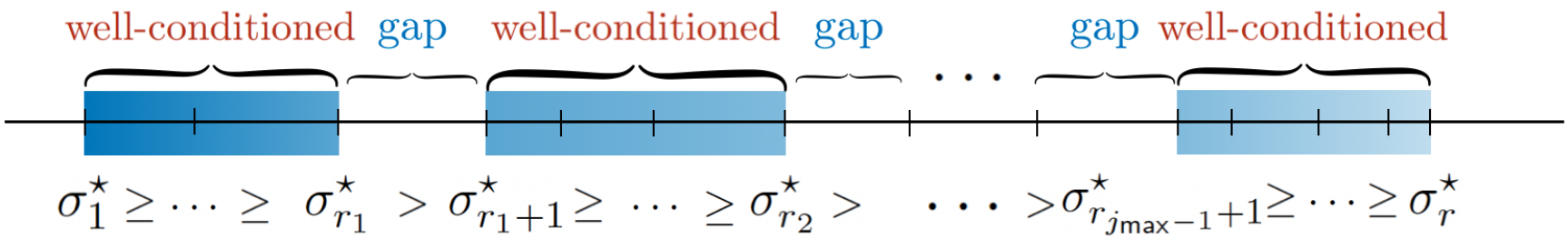


solution:

- divide eigenvalues into well-conditioned & well-separated subblocks
- estimate subblocks sequentially

Proposed algorithm: deflated-HeteroPCA



- sequentially choose ranks $\underbrace{r_0 = 0 < r_1 < \cdots < r_{j_{\max}} = r}_{\text{data-driven}}$ s.t.
  - $\sigma_{r_{j-1}+1}^\star / \sigma_{r_j}^\star$ is small
  - sufficient gap between $\sigma_{r_j}^\star$ and $\sigma_{r_j+1}^\star$

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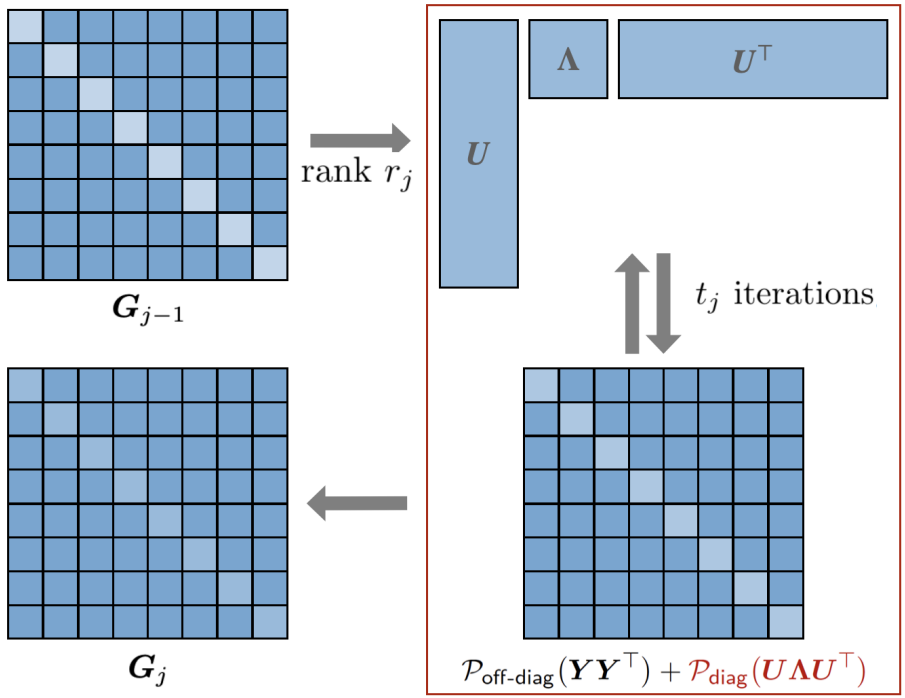

- sequentially choose ranks $\underbrace{r_0 = 0 < r_1 < \cdots < r_{j_{\max}} = r}_{\text{data-driven}}$ s.t.
  - $\sigma^\star_{r_{j-1}+1}/\sigma^\star_{r_j}$ is small
  - sufficient gap between $\sigma^\star_{r_j}$ and $\sigma^\star_{r_j+1}$
- invoke HeteroPCA($\underbrace{\boldsymbol{G}_{j-1}}_{\text{input}}, \underbrace{r_j}_{\text{rank}}$) to impute diagonals & obtain $\boldsymbol{G}_k$

Proposed algorithm: deflated-HeteroPCA

- **Initialize:** $\boldsymbol{G}^0 = \mathcal{P}_{\text{off-diag}}(\boldsymbol{Y}\boldsymbol{Y}^\top), k = 0, r_0 = 0$
- **Sequential updates:** while $r_k < r$

$$
\begin{aligned}
&j = j + 1 \\
&\text{select } r_j \text{ in a data-driven manner} \\
&(\boldsymbol{G}_j, \boldsymbol{U}_j) = \text{HeteroPCA}(\underbrace{\boldsymbol{G}_{j-1}}_{\text{input}}, \underbrace{r_j}_{\text{rank}})
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$$

- **Output:** $\boldsymbol{U} := \boldsymbol{U}_j \quad \longrightarrow \quad$ estimate of $\boldsymbol{U}^\star$

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$$\text{Select } r_j = \begin{cases} \max \mathcal{R}_j, & \text{if } \mathcal{R}_j \neq \emptyset, \\ r, & \text{otherwise.} \end{cases} \text{ Here,}$$

$$\mathcal{R}_j := \{r' : r_{j-1} < r' \leq r,\ \overbrace{\sigma_{r_{j-1}+1}(\boldsymbol{G}_{j-1}) / \sigma_{r'}(\boldsymbol{G}_{j-1}) \leq 4}^{\text{well-conditioned}} \ \& \ \underbrace{\sigma_{r'}(\boldsymbol{G}_{j-1}) - \sigma_{r'+1}(\boldsymbol{G}_{j-1}) \geq \sigma_{r'}(\boldsymbol{G}_{j-1})/r}_{\text{gap}}\}.$$

Performance of Deflated-HeteroPCA

Zhou, Chen '23a (informal):

Under essential assumptions on $\sigma_r^\star$ and regularity assumptions, Deflated-HeteroPCA

- can handle heteroskedastic noise
- enjoys near-optimal and condition-number-free guarantees

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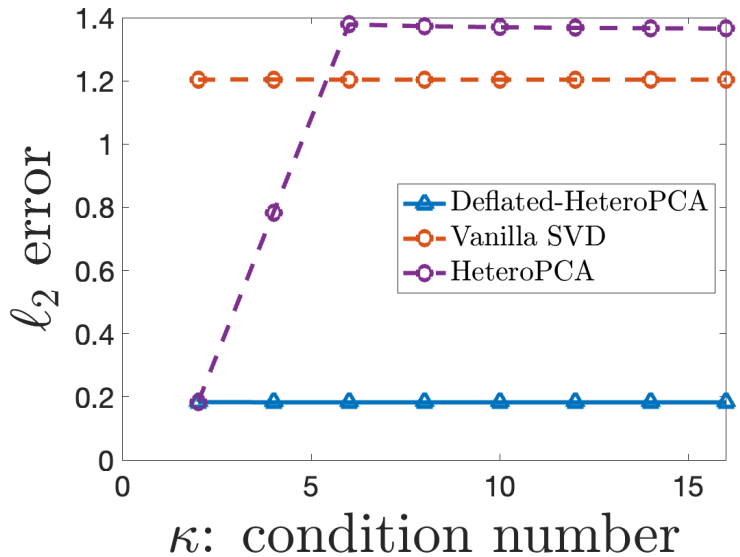

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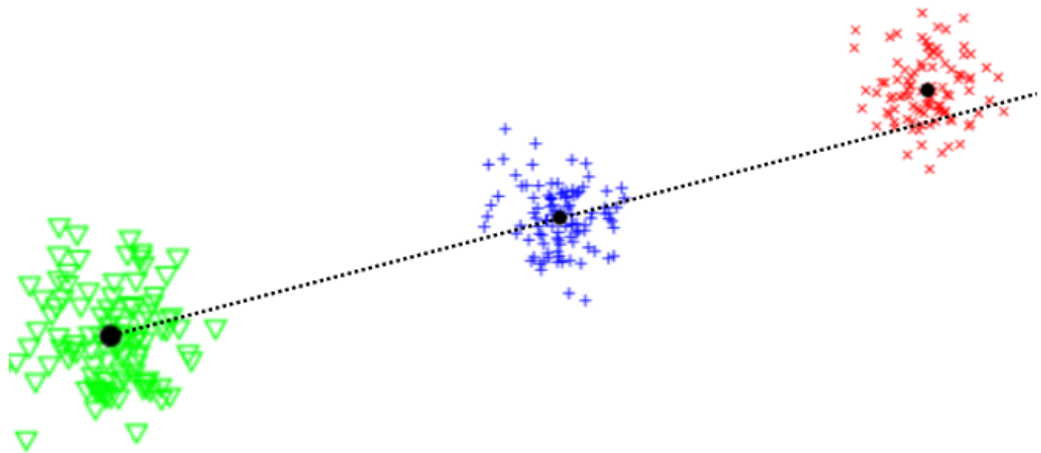

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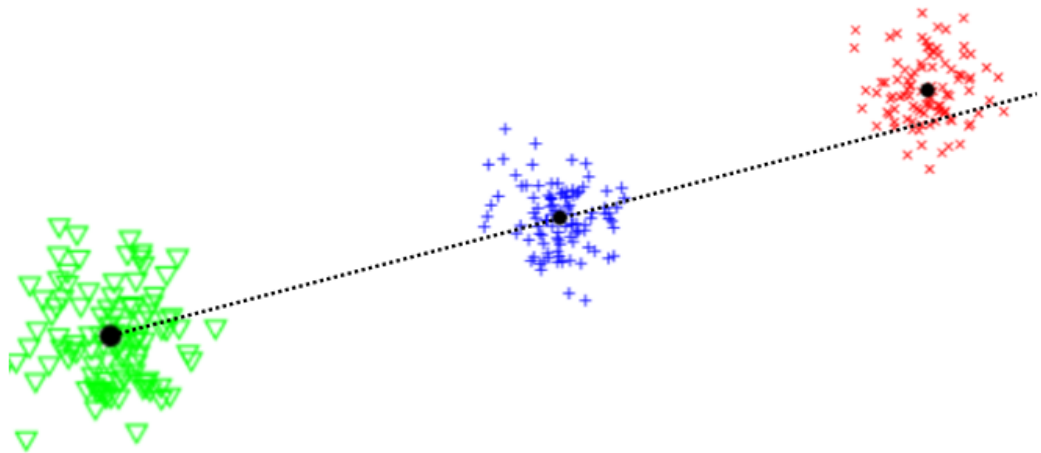

- Only large singular values matter! Add a thresholding procedure!

Thresholded Deflated-HeteroPCA$(\boldsymbol{Y}, r, \tau)$

- **Initialize:** $\boldsymbol{G}^0 = \mathcal{P}_{\text{off-diag}}(\boldsymbol{Y}\boldsymbol{Y}^\top), j = 0, r_0 = 0$
- **Sequential updates:** while $r_j < r$ and $\sigma_{r_j+1}(\boldsymbol{G}_j) > \underbrace{\tau}_{\substack{\text{data-driven} \\ \text{threshold}}}$

  $j = j + 1$

  select r_j in a data-driven manner

  $(\boldsymbol{G}_j, \boldsymbol{U}_j) = \text{HeteroPCA}(\boldsymbol{G}_{j-1}, r_j)$
- **Output:** $U := \boldsymbol{U}_j \quad \longrightarrow \quad$ estimate of $\boldsymbol{U}^\star$

Proposed algorithm: High-order HeteroClustering

- Step 1: estimate "important" subspaces of $\boldsymbol{X}_i^\star = \mathcal{M}_i(\boldsymbol{\mathcal{X}}^\star)$

  - Obtain $\boldsymbol{U}_i$ via Thresholded Deflated-HeteroPCA$(\boldsymbol{X}_i^\star, k_i, \tau)$

- Step 2: apply approximate k-means on the rows of

$$\widehat{\boldsymbol{B}}_i = \mathcal{M}_i(\boldsymbol{\mathcal{Y}} \underbrace{\times_i \boldsymbol{U}_i \boldsymbol{U}_i^\top}_{\text{denoising}} \underbrace{\times_{i+1} \boldsymbol{U}_{i+1} \times_{i+2} \boldsymbol{U}_{i+2}}_{\text{dimension reduction \& denoising}})$$

- Optional update: HLloyd (Han et al. '22)

Assumptions (ignoring log factors)

- dimension $n_1 \asymp n_2 \asymp n_3 \asymp n$
- **heteroskedasticity**: $\mathcal{E}$ has indep. zero-mean entries obeying
  - $\mathsf{Var}[E_{i,j,\ell}] \leq \omega_{\mathsf{max}}^2$
  - $|E_{i,j,\ell}| \lesssim \omega_{\mathsf{max}} n^{3/4}$ with high prob.
  - examples: sub-Gaussian, centered Poisson, STBM

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- balanced cluster sizes: $\left|\left\{j \in [n_i] : \left(\boldsymbol{z}_i^\star\right)_j = \ell\right\}\right| \asymp n_i/k_i$
- number of clusters $k_i = O(1)$

Theoretical guarantees

Theorem 1 (Zhou, Chen '23)

Assume that either (1) or (2) is satisfied:

(1). *noise is not too spiky (e.g.,* $\mathsf{Var}\left[E_{i,j,\ell}\right] \asymp \omega_{\mathsf{max}}^2$*);*

(2). *The observation model is STBM.*

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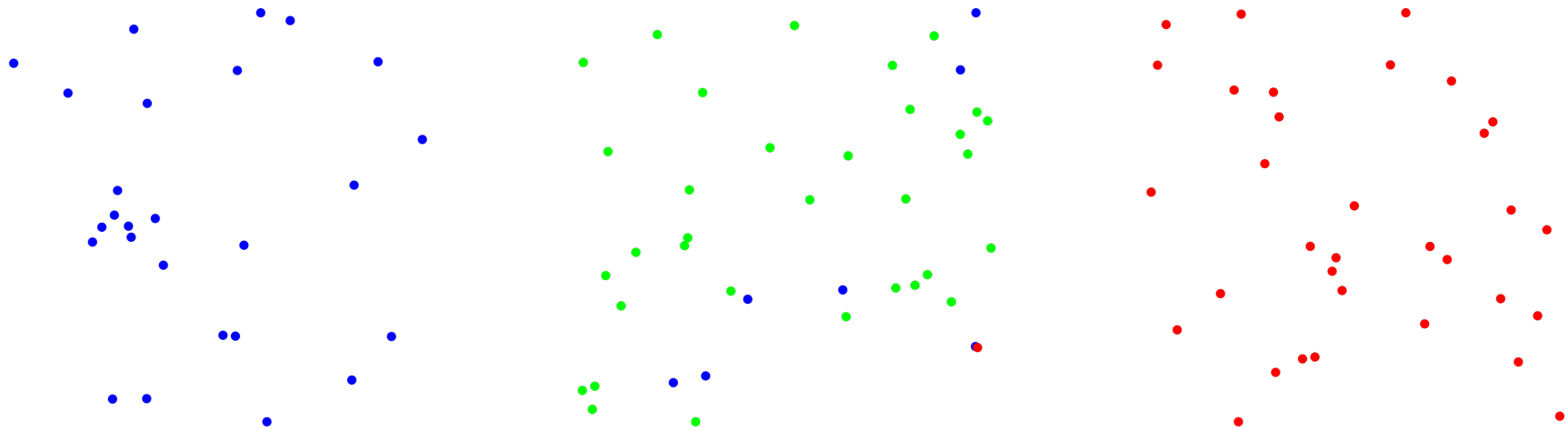
W.h.p., HHC and HHC + HLloyd achieve exact clustering.

- (almost) necessary SNR condition among poly-time algorithms
- handle heteroskedastic noise & no superfluous assumptions on $\boldsymbol{\mathcal{S}}^\star$

Numerical experiments

The toy example



HHC

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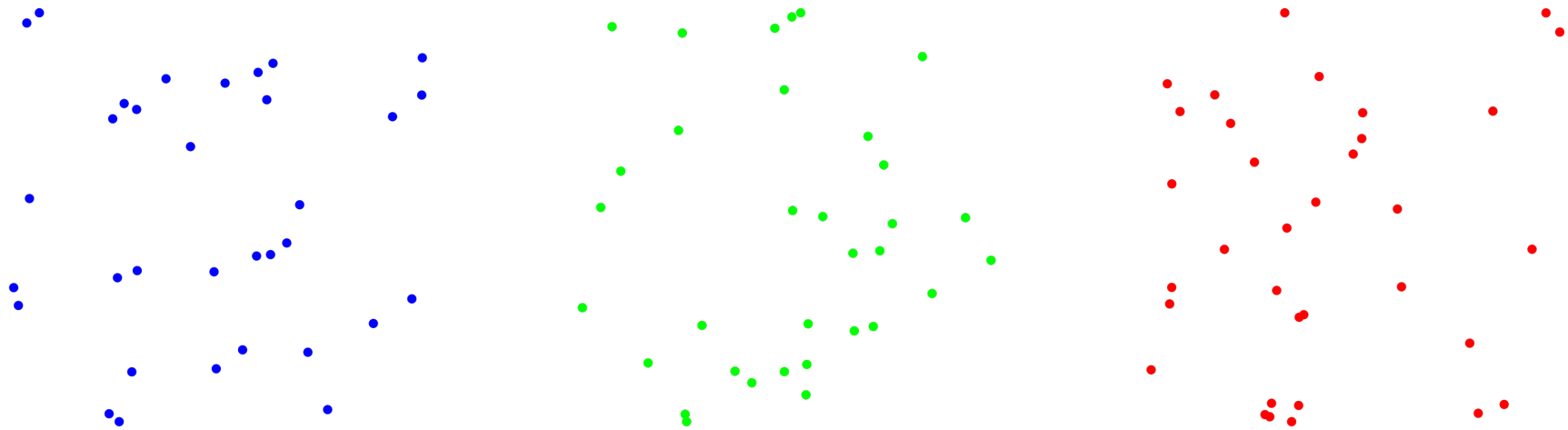

HHC + HLloyd

Real data example: the flight route network

- OpenFlights Airports Database: global fight information*
- top 50 airports based on the number of flights $\rightarrow$ 39 airlines†
- data $\boldsymbol{\mathcal{Y}} \in \{0,1\}^{39\times 50\times 50}$:

$$Y_{i,j,\ell} = \begin{cases} 1, & \text{if airline } i \text{ operates a flight route b/w airports } j, \ell, \\ 0, & \text{otherwise.} \end{cases}$$

*original data: `https://openflights.org/data`

†processed data: `https://github.com/Rungang/HLloyd/blob/master/experiment/flight_route.RData`

Real data example: the flight route network

Select the clustering sizes based on BIC: $(k_1, k_2, k_3) = (5, 5, 5)$

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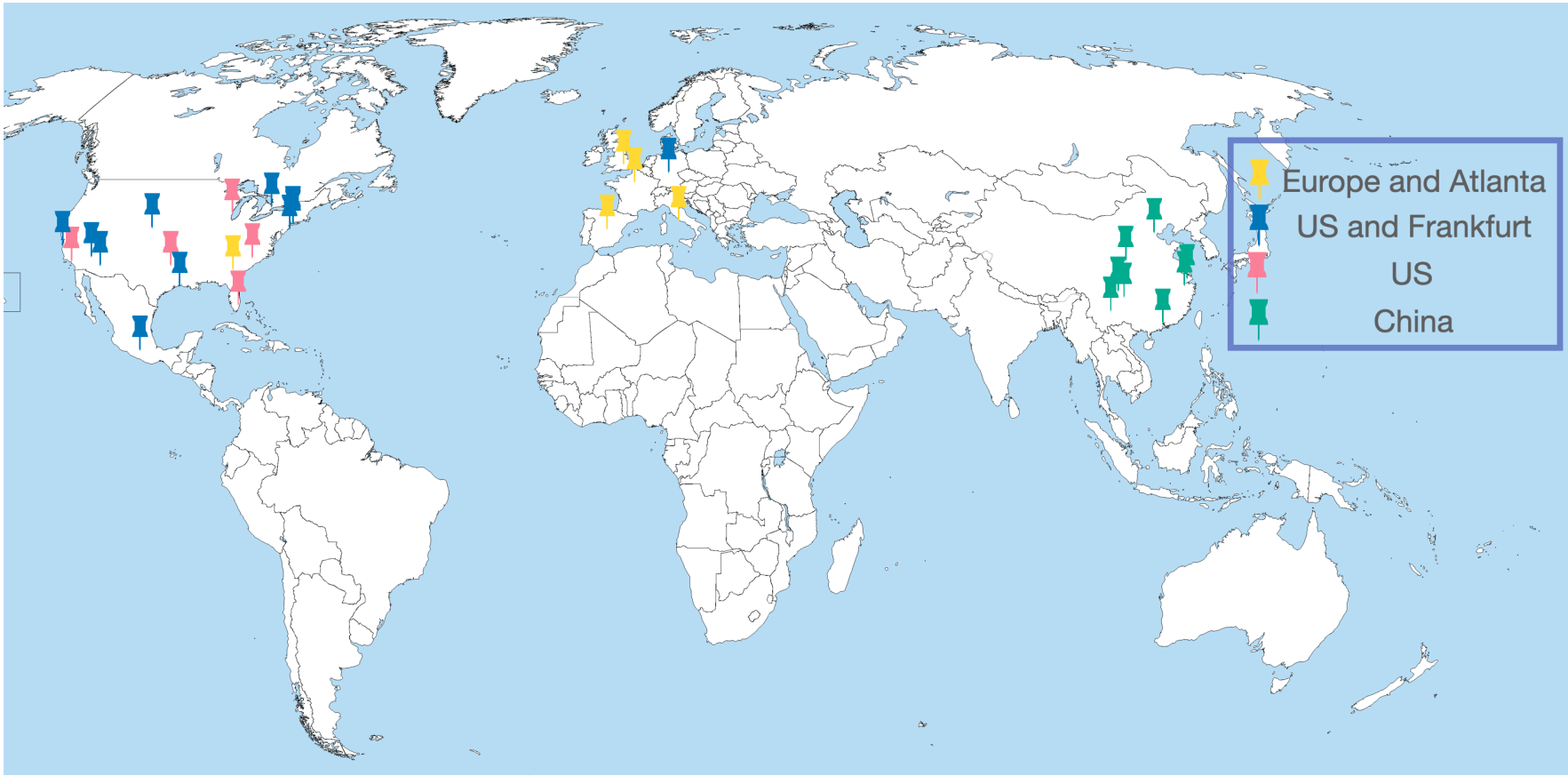

Ours

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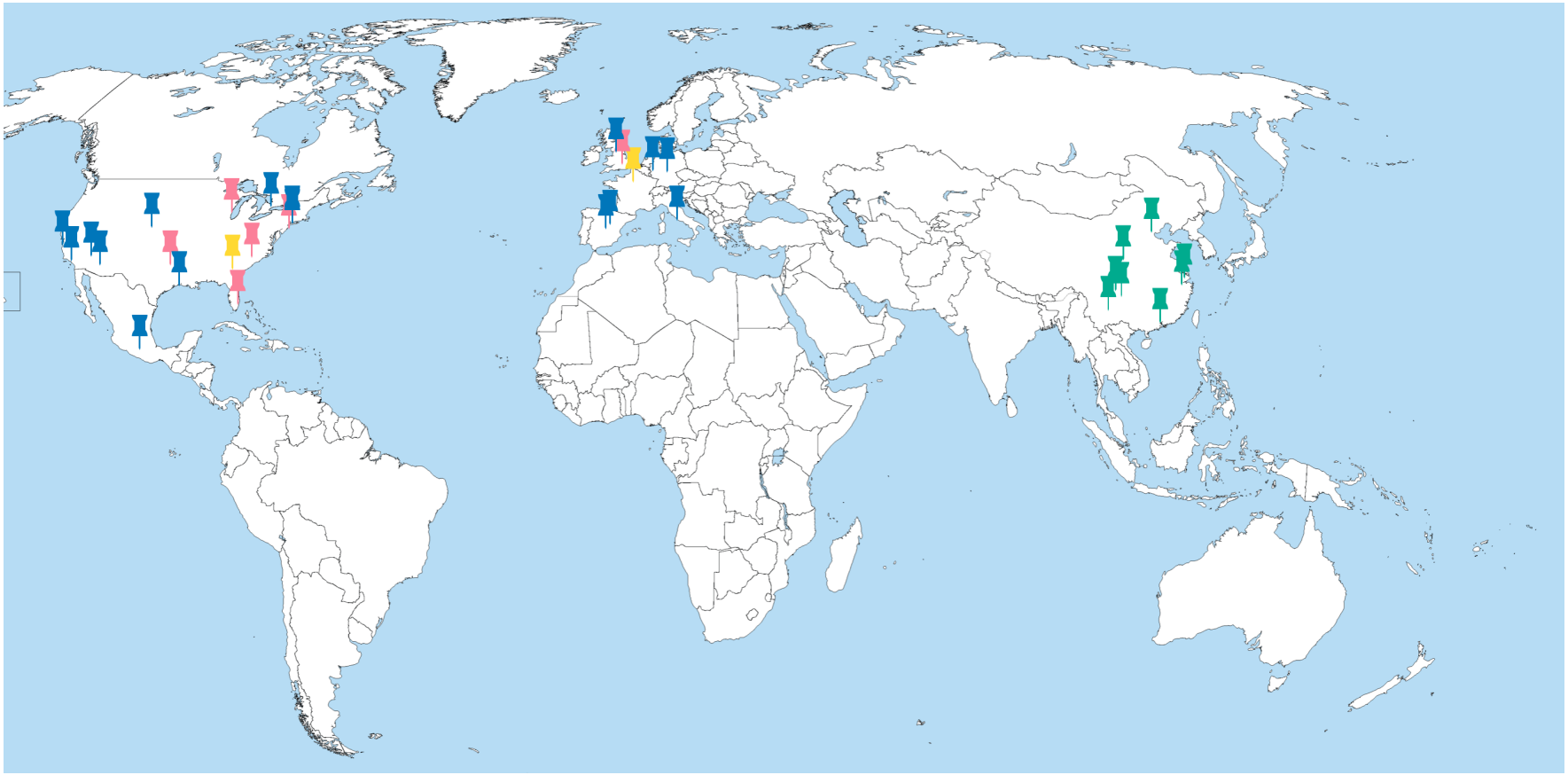

Han et al.'22

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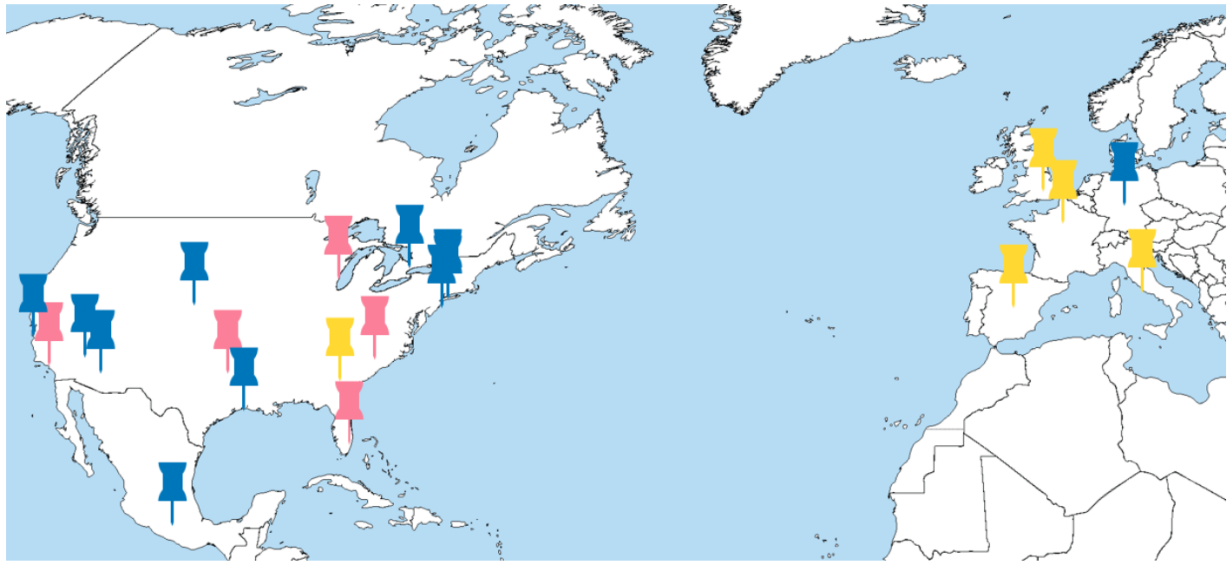
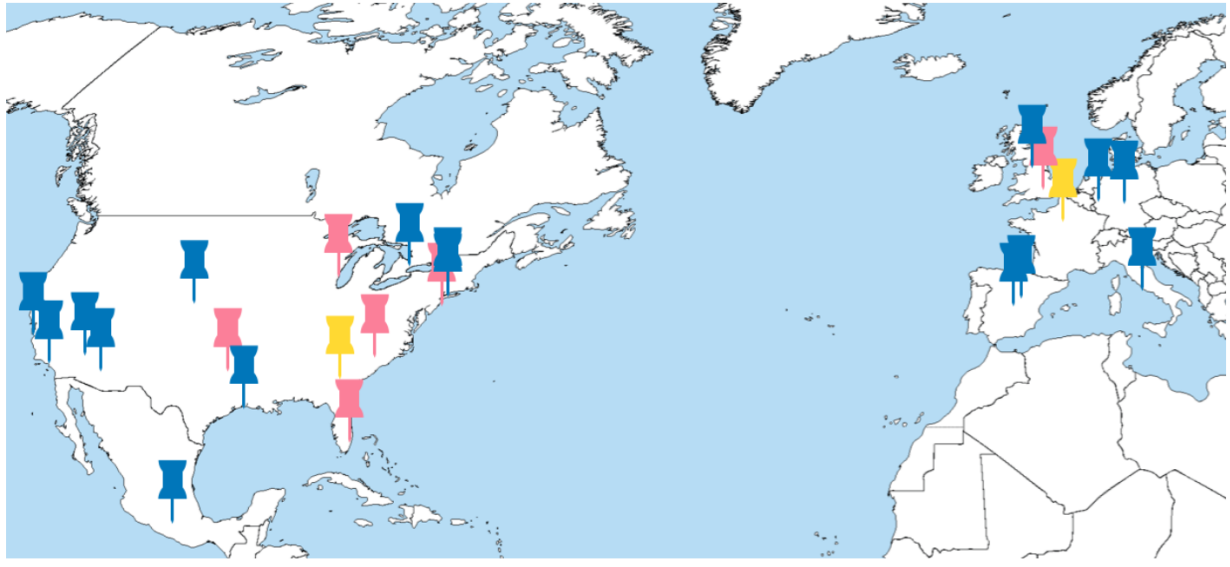
Ours



Han et al.'22



A glimpse of proof highlights

- Crucial step: controlling each row of $(\boldsymbol{I} - \boldsymbol{U}_i \boldsymbol{U}_i^\top)\mathcal{M}_i(\boldsymbol{\mathcal{X}}^\star)$
  - need sharp and condition-number-free guarantees w/o least singular value and condition number restrictions

- **New technique**: bounding an infinite sum of $\ell_{2,\infty}$ norms of error polynomials instead

- careful induction analyses for error polynomials

Summary

Tensor clustering: a novel method that

- can handle heteroskedastic noise
- achieves exact clustering if SNR exceeds computational limit

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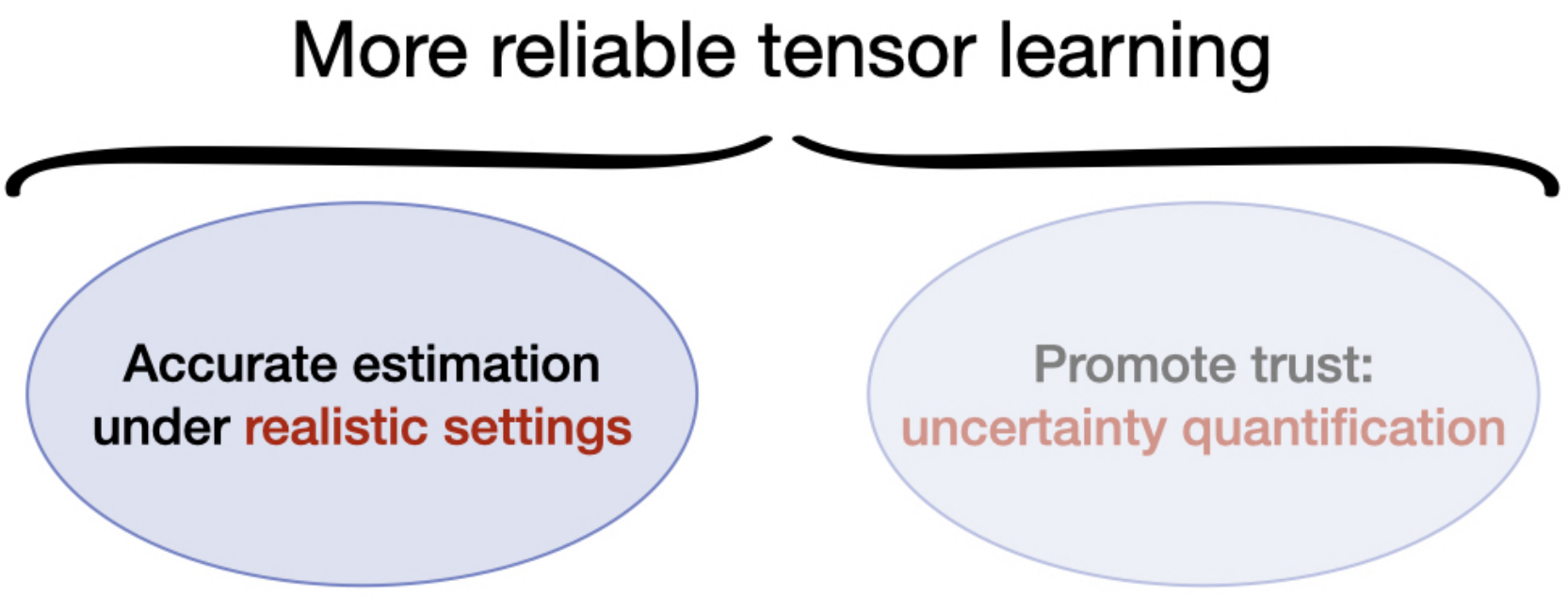
papers:

Y. Zhou, Y. Chen, "Deflated HeteroPCA: Overcoming the Curse of Ill-conditioning in Heteroskedastic PCA," under review at *Annals of Statistics*

Y. Zhou, Y. Chen, "Heteroskedastic Tensor Clustering,"under review at *JRSSB*


More reliable tensor learning
Accurate estimation
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Promote trust:
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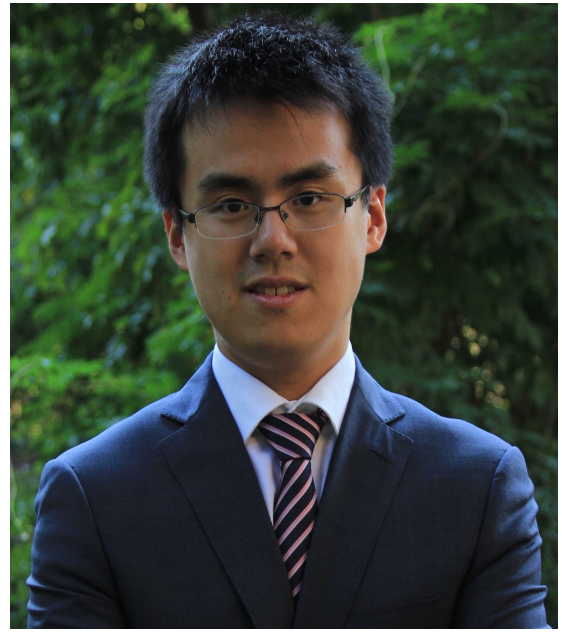
Part 2:
Uncertainty quantification for tensor learning

Dong Xia
HKUST



Anru Zhang
Duke University

Uncertainty Quantification for Tensor Learning?

- Many methods on low-rank tensor estimation
  - tensor PCA
  - tensor clustering
  - tensor regression
  - ...

Uncertainty Quantification for Tensor Learning?

- Many methods on low-rank tensor estimation
  - tensor PCA
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- **The statistical inference or uncertainty quantification** for low-rank tensor models remains largely unexplored!

Uncertainty Quantification for Tensor Learning?

We focus on

- inference of principal components of Tucker low-rank tensors under tensor PCA model

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Covered in the paper but not the talk:

- entry-wise inference for rank-1 tensors
- inference of principal components of Tucker low-rank tensors under tensor regression model

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Covered in the paper but not the talk:

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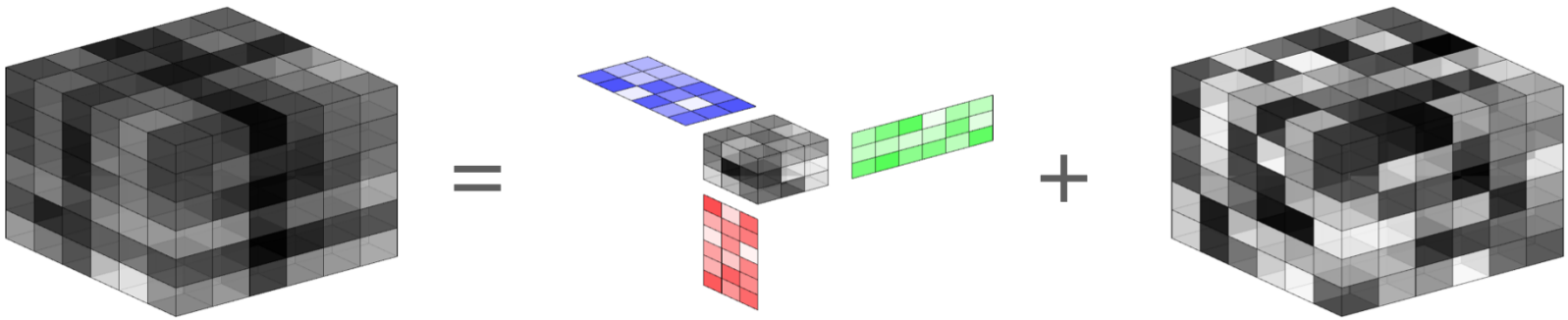
First inference results for Tucker low-rank tensors!

Inference for Tucker low-rank tensor PCA

Tensor PCA model: Observe

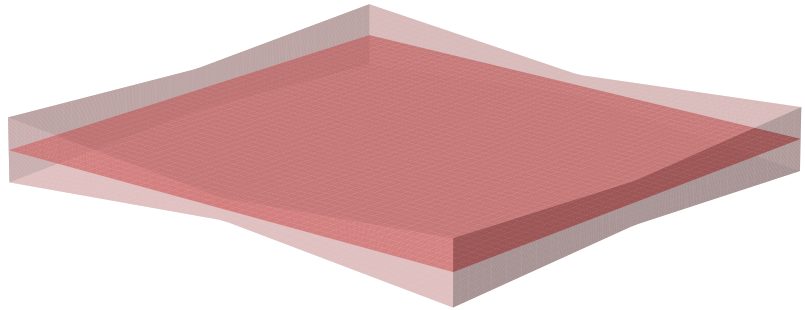
$$\boldsymbol{\mathcal{A}} = \boldsymbol{\mathcal{T}}^\star + \boldsymbol{\mathcal{Z}} \in \mathbb{R}^{n_1 \times n_2 \times n_3}, \tag{2}$$

where the signal $\boldsymbol{\mathcal{T}}^\star = \boldsymbol{\mathcal{S}}^\star \times_1 \boldsymbol{U}_1^\star \times_2 \boldsymbol{U}_2^\star \times_3 \boldsymbol{U}_3^\star$ and the noise $\boldsymbol{\mathcal{Z}}$ contains i.i.d. entries $N(0, \omega^2)$.

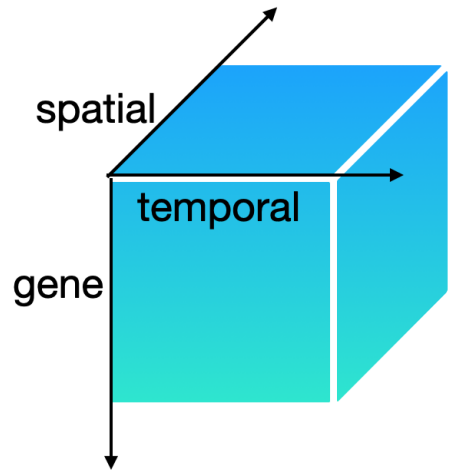


Inference for Tucker low-rank tensor PCA

Goal: Inference for $\{\boldsymbol{U}_i^\star\}_{i=1}^3$



- Spatial and temporal patterns of gene regulation during brain development (Liu et al. '17)



- Hidden components in Gaussian mixture models (Anandkumar et al. '14)

Estimation

- Least squares estimator:

$$\widehat{\boldsymbol{\mathcal{T}}} = \underset{\mathsf{rank}(\boldsymbol{\mathcal{T}}) \leq (r_1, r_2, r_3)}{\arg\min} \|\boldsymbol{\mathcal{T}} - \boldsymbol{\mathcal{A}}\|_{\mathrm{F}}^2$$

$$\iff (\widehat{\boldsymbol{U}_1}, \widehat{\boldsymbol{U}_2}, \widehat{\boldsymbol{U}_3}) = \underset{\boldsymbol{U}_j \in \mathbb{O}_{n_j, r_j}}{\arg\max} \|\boldsymbol{\mathcal{A}} \times_1 \boldsymbol{U}_1^\top \times_2 \boldsymbol{U}_2^\top \times_3 \boldsymbol{U}_3^\top\|_{\mathrm{F}}^2.$$

Highly non-convex!

- High-order orthogonal iteration (HOOI, De Lathauwer et al. '00): alternating minimization

High-order orthogonal iteration (HOOI)

- **Spectral initialization:** $\widehat{\boldsymbol{U}}_i^{(0)}$, $1 \le i \le 3$
- **Sequential updates:** for $t = 0, 1, \ldots, t_{\mathsf{max}}$

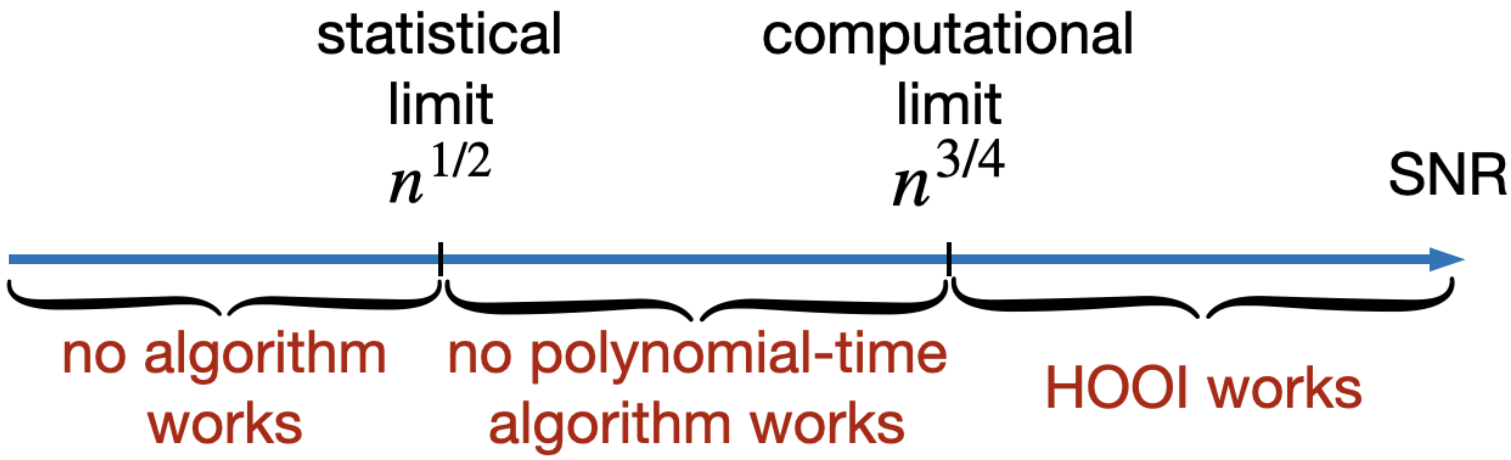
$$\widehat{\boldsymbol{U}}_1^{(t)} = \mathsf{SVD}_{r_1}\left(\mathcal{M}_1\left(\boldsymbol{\mathcal{A}} \times_2 \widehat{\boldsymbol{U}}_2^{(t-1)\top} \times_3 \widehat{\boldsymbol{U}}_3^{(t-1)\top}\right)\right).$$

Update $\widehat{\boldsymbol{U}}_2^{(t)}$ and $\widehat{\boldsymbol{U}}_3^{(t)}$ similarly

- **Output:** $\widehat{\boldsymbol{U}}_i := \widehat{\boldsymbol{U}}_i^{(t_{\mathsf{max}})} \longrightarrow$ estimate of $\boldsymbol{U}_i^\star$

$$\widehat{\boldsymbol{\mathcal{S}}} := \boldsymbol{\mathcal{A}} \times_1 \widehat{\boldsymbol{U}}_1^\top \times_2 \widehat{\boldsymbol{U}}_2^\top \times_3 \widehat{\boldsymbol{U}}_3^\top \longrightarrow \text{estimate of } \boldsymbol{\mathcal{S}}^\star$$

Statistical-computational gap



signal strenth $\lambda^\star_{\min} := \lambda_{\min}(\boldsymbol{\mathcal{T}}^\star) = \min_j \sigma_{r_j}\left(\mathcal{M}_j(\boldsymbol{\mathcal{T}}^\star)\right)$

noise level $\omega :=$ standard deviation of entries of $\boldsymbol{\mathcal{Z}}$

SNR $:= \lambda^\star_{\min}/\omega$

Inference for Tucker Low-rank Tensor PCA

- How to make inference?

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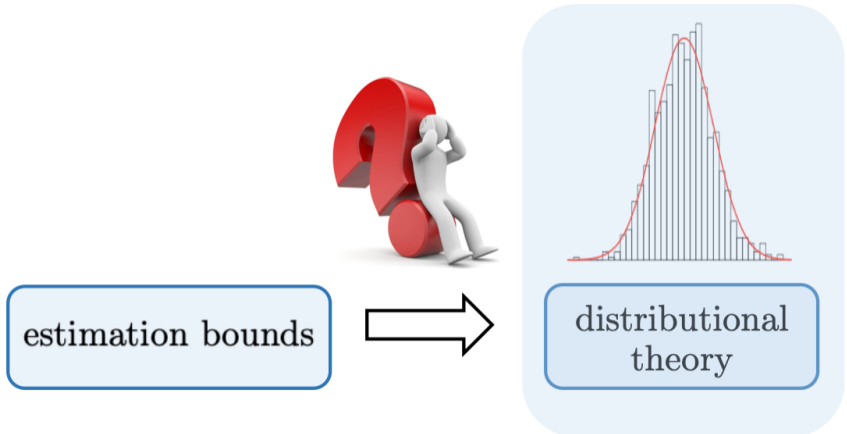
- How to make inference?
- Most existing statistical inference methods are for **global minimizers of convex problems**
  - MLE
  - sparse linear regression
  - matrix completion
  - matrix regression

Inference for Tucker Low-rank Tensor PCA

- How to make inference?
- Most existing statistical inference methods are for **global minimizers of convex problems**
- **Challenge**: distribution theory for subspace estimates from non-convex iterations under essential SNR assumption



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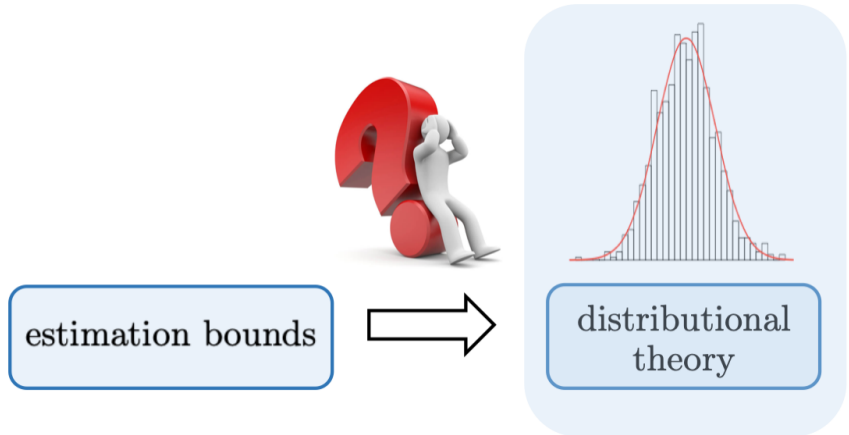

- A slightly stronger SNR condition enables us to make inference!

Two-iteration algorithm for inference

- **Input:** Rate-optimal estimators $\widehat{\boldsymbol{U}}_1^{(0)}, \widehat{\boldsymbol{U}}_2^{(0)}, \widehat{\boldsymbol{U}}_3^{(0)}$
- **Sequential updates:** for $t = 0, 1$

$$\widehat{\boldsymbol{U}}_1^{(t+1)} = \mathsf{SVD}_{r_1}\left(\mathcal{M}_1\left(\boldsymbol{\mathcal{A}} \times_2 \widehat{\boldsymbol{U}}_2^{(t)\top} \times_3 \widehat{\boldsymbol{U}}_3^{(t)\top}\right)\right)$$
$$\widehat{\boldsymbol{U}}_2^{(t+1)} = \mathsf{SVD}_{r_2}\left(\mathcal{M}_2\left(\boldsymbol{\mathcal{A}} \times_3 \widehat{\boldsymbol{U}}_3^{(t)\top} \times_1 \widehat{\boldsymbol{U}}_1^{(t)\top}\right)\right)$$
$$\widehat{\boldsymbol{U}}_3^{(t+1)} = \mathsf{SVD}_{r_3}\left(\mathcal{M}_3\left(\boldsymbol{\mathcal{A}} \times_1 \widehat{\boldsymbol{U}}_1^{(t)\top} \times_2 \widehat{\boldsymbol{U}}_2^{(t)\top}\right)\right)$$

- **Output:** Final estimates $\widehat{\boldsymbol{U}}_1 := \widehat{\boldsymbol{U}}_1^{(2)}, \widehat{\boldsymbol{U}}_2 := \widehat{\boldsymbol{U}}_2^{(2)}, \widehat{\boldsymbol{U}}_3 := \widehat{\boldsymbol{U}}_3^{(2)}$, $\widehat{\boldsymbol{\mathcal{G}}} := \boldsymbol{\mathcal{A}} \times_1 \widehat{\boldsymbol{U}}_1^\top \times_2 \widehat{\boldsymbol{U}}_2^\top \times_3 \widehat{\boldsymbol{U}}_3^\top$

Theoretical guarantees

Theorem 2 (Xia, Zhang, Zhou '22)

Suppose $n_j \asymp n$ *and* $\lambda^\star_{\min}/\omega \gg n^{3/4}$. *Under regularity assumptions,*

$$\|\sin\Theta(\widehat{\boldsymbol{U}}_j, \boldsymbol{U}_j^\star)\|_{\mathrm{F}}^2 \sim N(mean, variance) + \text{ negligible terms.}$$

- $mean = n_j\omega^2\|\boldsymbol{\Lambda}_j^{\star -1}\|_{\mathrm{F}}^2$
- $variance = \sqrt{2n_j}\omega^2\|\boldsymbol{\Lambda}_j^{\star -2}\|_{\mathrm{F}}$
- $\boldsymbol{\Lambda}_j^\star$: *diagonal matrix containing the singular values of* $\mathcal{M}_j(\boldsymbol{\mathcal{T}}^\star)$.

$$\|\sin\Theta(\widehat{\boldsymbol{U}}_j^{(0)}, \boldsymbol{U}_j^\star)\|_{\mathrm{F}} = \sqrt{r_j - \sum_{i=1}^{r_j}\sigma_i^2(\boldsymbol{U}_j^{\star\top}\widehat{\boldsymbol{U}}_j^{(0)})}.$$

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- SNR condition $\lambda^\star_{\min}/\omega \gg n^{3/4}$ is slighter stronger than the one for estimation ($\lambda^\star_{\min}/\omega \gtrsim n^{3/4}$)

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$$\frac{\|\sin\Theta(\widehat{\boldsymbol{U}}_j, \boldsymbol{U}_j^\star)\|_{\mathrm{F}}^2 - n_j\widehat{\omega}^2\|\widehat{\boldsymbol{\Lambda}}_j^{-1}\|_{\mathrm{F}}^2}{\sqrt{2n_j}\widehat{\omega}^2\|\widehat{\boldsymbol{\Lambda}}_j^{-2}\|_{\mathrm{F}}} \sim N(0,1) + \textit{ negligible terms.}$$

Here, $\widehat{\boldsymbol{\Lambda}}_j$ and $\widehat{\omega}$ are data-driven estimates for $\boldsymbol{\Lambda}_j^\star$ and ω, respectively.

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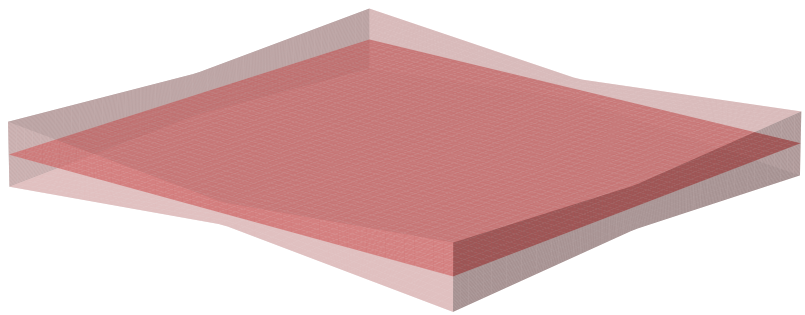
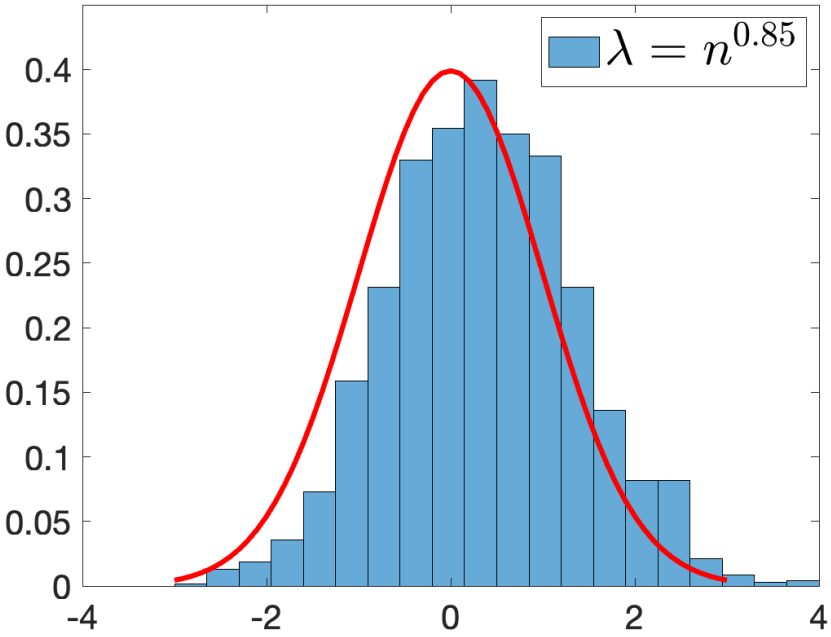
Here, $\widehat{\boldsymbol{\Lambda}}_j$ and $\widehat{\omega}$ are data-driven estimates for $\boldsymbol{\Lambda}_j^\star$ and ω, respectively.

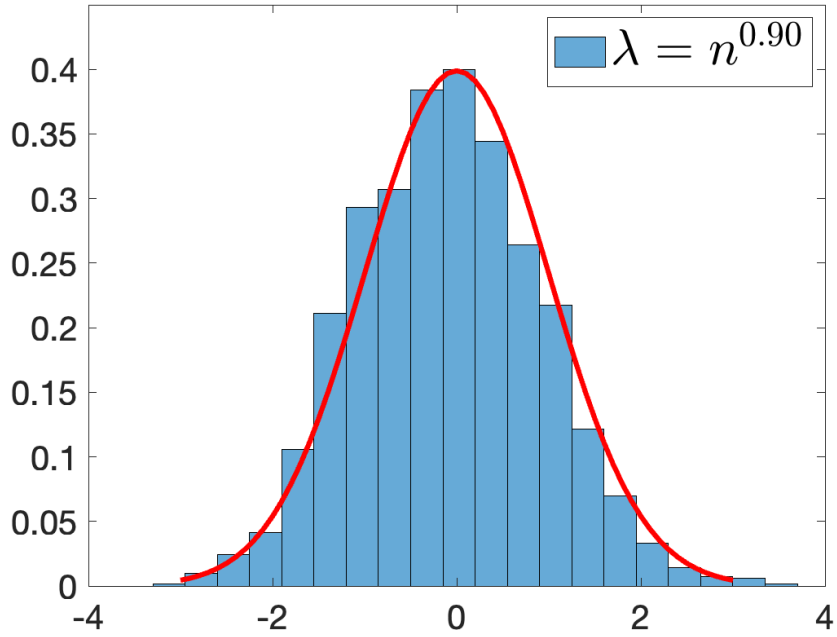
$(1-\alpha)$-level confidence region for $\boldsymbol{U}_j^\star$: Let $z_\alpha = \Phi^{-1}(1-\alpha)$,

$$\mathrm{CR}_\alpha(\widehat{\boldsymbol{U}}_j) := \left\{\boldsymbol{V} \in \mathbb{O}_{n_j,r_j} : \|\sin\Theta(\widehat{\boldsymbol{U}}_j, \boldsymbol{V})\|_{\mathrm{F}}^2 \le n_j\widehat{\omega}^2\|\widehat{\boldsymbol{\Lambda}}_j^{-1}\|_{\mathrm{F}}^2 + z_\alpha\sqrt{2n_j}\widehat{\omega}^2\|\widehat{\boldsymbol{\Lambda}}_j^{-2}\|_{\mathrm{F}}\right\}.$$



Numerical simulations





Normal approximation of $\dfrac{\|\sin\Theta(\widehat{\boldsymbol{U}}_j,\boldsymbol{U}_j^\star)\|_{\mathrm{F}}^2 - n_j\widehat{\omega}^2\|\widehat{\boldsymbol{\Lambda}}_j^{-1}\|_{\mathrm{F}}^2}{\sqrt{2n_j}\widehat{\omega}^2\|\widehat{\boldsymbol{\Lambda}}_j^{-2}\|_{\mathrm{F}}}$

$n_1 = n_2 = n_3 = n = 200$, $r = 3$, and $\omega = 1$

Summary

- Two-iteration algorithm for inference

- The inference of principle components can be efficiently done when a computationally feasible optimal estimate is achievable!

paper:

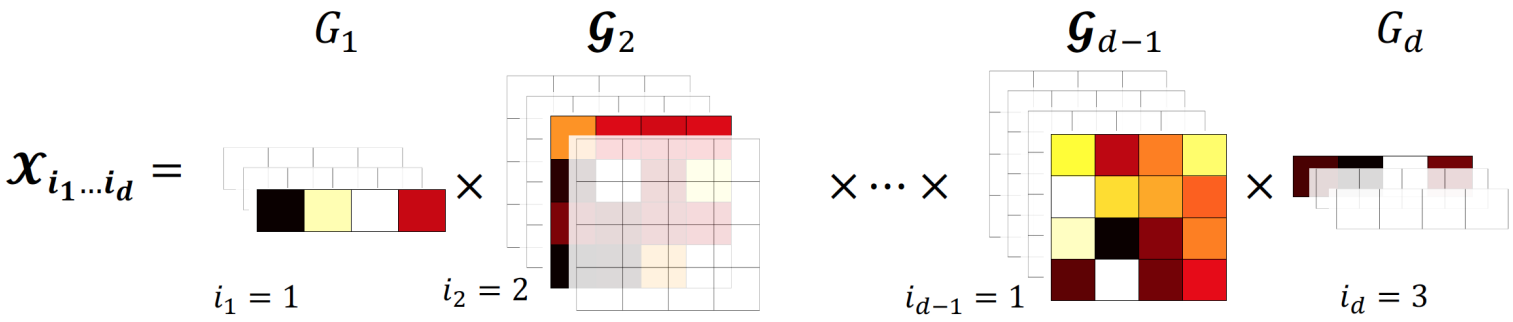
D. Xia, A. Zhang, Y. Zhou, "Inference for Low-rank Tensors – No Need to Debias," *Annals of Statistics*, 2022

Highlight of my research

For modern statistical problems:

- design efficient and statistically accurate algorithms
- establish theoretical foundations

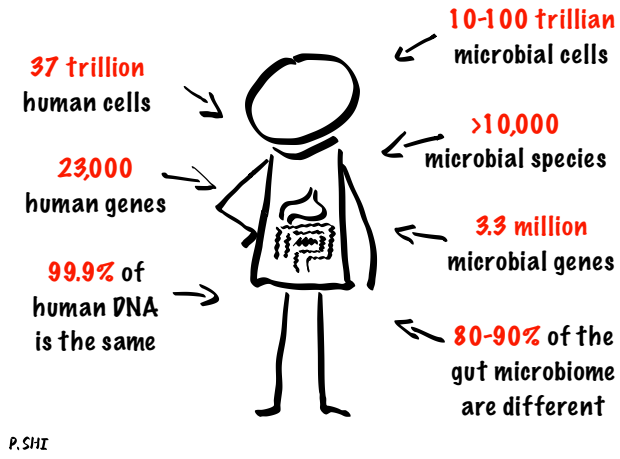
High-order tensor SVD

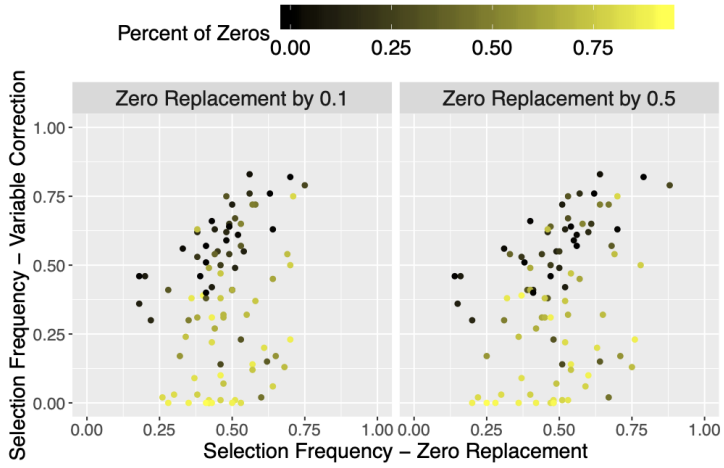


- Novel method: tensor-train orthogonal iteration (TTOI)
- Theory: *minimax optimal* estimation error

Y. Zhou, A. Zhang, L. Zheng, Y. Wang, "Optimal High-Order Tensor SVD via Tensor-Train Orthogonal Iteration," *IEEE Transactions on Information Theory*, 2022

Microbial compositional data

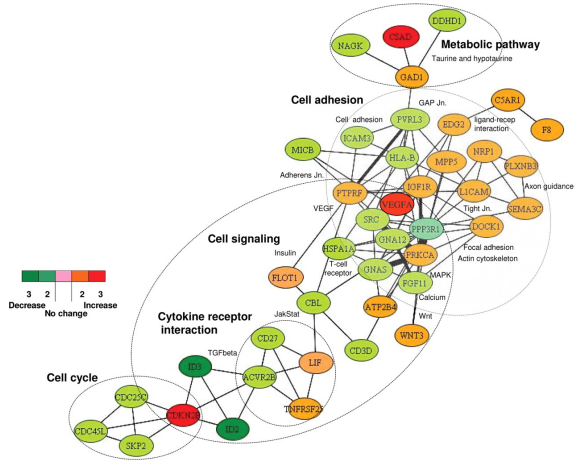




- Goal: Identifying microbial taxa or genes associated with clinical phenotypes
- Propose log-error-in-variable model & new method
- Theory: optimal guarantee for estimation error

P. Shi, Y. Zhou, A. Zhang, "High-dimensional Log-Error-in-Variable Regression with Applications to Microbial Compositional Data Analysis," *Biometrika*, 2022

Double sparse regression



- Theory: sparse group Lasso achieves optimal estimation guarantees

- Multi-objective regularizers can help!

T. Cai, A. Zhang, Y. Zhou, "Sparse Group Lasso: Optimal Sample Complexity, Convergence Rate, and Statistical Inference ," *IEEE Transactions on Information Theory*, 2022

Future directions

- Tensor problems under more realistic assumptions
- Federated statistical learning
- Theoretical foundations of deep learning
- ...

Thank you!

Assumptions (ignoring log factors)

- **heteroskedasticity**: $E'_{i,j}s$ are indep. obeying
  - $\mathbb{E}[E_{i,j}] = 0, \qquad \mathsf{Var}\,[E_{i,j}] \leq \omega^2$
  - $|E_{i,j}| \lesssim \omega \min\left\{ (n_1 n_2)^{1/4}, \sqrt{n_2} \right\}$ with high prob.
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- rank $r = O(1)$
- incoherence $\mu := \max\{ \frac{n_1}{r} \left\| \boldsymbol{U}^\star \right\|_{2,\infty}^2, \frac{n_2}{r} \left\| \boldsymbol{V}^\star \right\|_{2,\infty}^2 \} = O(1)$

Theoretical guarantees

Theorem 3 (Zhou, Chen '23)

With high prob., Deflated-HeteroPCA yields

$$\|\boldsymbol{U}\boldsymbol{R}_{\boldsymbol{U}} - \boldsymbol{U}^{\star}\| \lesssim \zeta_{\mathsf{op}}$$

for some rotation matrix $\boldsymbol{R}_{\boldsymbol{U}}$*, where* $\zeta_{\mathsf{op}} = \frac{\sqrt{n_1 n_2}\,\omega^2}{\sigma_r^{\star 2}} + \frac{\sqrt{n_1}\,\omega}{\sigma_r^{\star}}$

- match minimax lower bounds in Zhang et al. '22 & Cai et al. '21
- condition-number-free

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Estimates for $\mathbf{\Lambda}_j^\star$ and ω^2

$\widehat{\mathbf{\Lambda}}_j$: diagonal matrix containing the top r_j singular values of

$$\mathcal{M}_j(\boldsymbol{\mathcal{A}} \times_{j+1} \widehat{\boldsymbol{U}}_{j+1}^\top \times_{j+2} \widehat{\boldsymbol{U}}_{j+2}^\top),$$

$$\widehat{\omega} = \|\boldsymbol{\mathcal{A}} - \underbrace{\boldsymbol{\mathcal{A}} \times_1 \widehat{\boldsymbol{U}}_1\widehat{\boldsymbol{U}}_1^\top \times_2 \widehat{\boldsymbol{U}}_2\widehat{\boldsymbol{U}}_2^\top \times_3 \widehat{\boldsymbol{U}}_3\widehat{\boldsymbol{U}}_3^\top}_{\approx \mathcal{T}}\|_{\mathrm{F}}/\sqrt{n_1n_2n_3}.$$

Theorem 4 (Xia, Zhang, Zhou '22)

$$\frac{\|\sin\Theta(\widehat{\boldsymbol{U}}_j, \boldsymbol{U}_j^\star)\|_{\mathrm{F}}^2 - n_j\widehat{\omega}^2\|\widehat{\mathbf{\Lambda}}_j^{-1}\|_{\mathrm{F}}^2}{\sqrt{2n_j}\widehat{\omega}^2\|\widehat{\mathbf{\Lambda}}_j^{-2}\|_{\mathrm{F}}} \sim N(0,1) + \textit{ negligible terms.}$$

Entry-wise Inference for Rank-1 Tensors

Model: Observe

$$\boldsymbol{\mathcal{A}} = \boldsymbol{\mathcal{T}}^\star + \boldsymbol{\mathcal{Z}}, \quad \boldsymbol{\mathcal{T}}^\star = \lambda^\star \cdot \boldsymbol{u}^\star \otimes \boldsymbol{v}^\star \otimes \boldsymbol{w}^\star.$$

Here, $\boldsymbol{u}^\star \in \mathbb{S}^{n_1-1}, \boldsymbol{v}^\star \in \mathbb{S}^{n_2-1}, \boldsymbol{w}^\star \in \mathbb{S}^{n_3-1}$, the singular value $\lambda^\star > 0$, and $\mathcal{Z} \overset{i.i.d.}{\sim} N(0, \omega^2)$.

Goal: Inference for $T^\star_{i,j,k}$

Entry-wise Inference for Rank-1 Tensors

Theorem 5

Suppose $\lambda^\star/\omega \gg n^{3/4}$. *Apply HOOI with* $t_{\mathsf{max}} \geq C_1 \log n$. *If* $|u_i^\star|, |v_j^\star|, |w_k^\star| \ll \min\{\lambda^\star/(n\omega), 1\}$, *then*

$$\Big(\frac{\lambda}{\omega}(\widehat{u}_i - u_i^\star),\ \frac{\lambda}{\omega}(\widehat{v}_j - v_j^\star),\ \frac{\lambda}{\omega}(\widehat{w}_k - w_k^\star)\Big)^\top \xrightarrow{\mathrm{d}} N(0, I_3) \quad \text{as} \quad p \to \infty.$$

If $\omega/\lambda^\star \ll |u_i^\star|, |v_j^\star|, |w_k^\star| \ll \min\{\lambda^\star/(n\omega), 1/\sqrt{\log n}\}$, *then*

$$\frac{\widehat{\mathcal{T}}_{ijk} - \mathcal{T}_{ijk}}{\widehat{\omega}\sqrt{\widehat{u}_i^2\widehat{v}_j^2 + \widehat{v}_j^2\widehat{w}_k^2 + \widehat{w}_k^2\widehat{u}_i^2}} \xrightarrow{\mathrm{d}} N(0,1) \quad \text{as} \quad n \to \infty.$$

Entry-wise Inference for Rank-1 Tensors

- upper bound conditions on $|u_i^\star|, |v_j^\star|, |w_k^\star|$ are weaker than the incoherence condition
- lower bound condition is essential for asymptotic normality: if $u_i^\star = v_j^\star = w_k^\star = 0$, then

$$\frac{\lambda^2 \widehat{\mathcal{T}}_{ijk}}{\omega^3} \xrightarrow{\mathrm{d}} G_1 G_2 G_3 \quad \text{as } n \to \infty, \quad (G_1, G_2, G_3)^\top \sim N(0, I_3).$$

- Asymptotic $(1-\alpha)$ confidence interval for $\mathcal{T}_{ijk}$:
$[\widehat{\mathcal{T}}_{ijk} - z_{\alpha/2}\sigma\sqrt{\widehat{u_i^2}\widehat{v_j^2} + \widehat{v_j^2}\widehat{w_k^2} + \widehat{w_k^2}\widehat{u_i^2}}, \widehat{\mathcal{T}}_{ijk} + z_{\alpha/2}\sigma\sqrt{\widehat{u_i^2}\widehat{v_j^2} + \widehat{v_j^2}\widehat{w_k^2} + \widehat{w_k^2}\widehat{u_i^2}}]$.