Estimating Shared Subspace with AJIVE: Power and Limitation of Multiple Data Matrices

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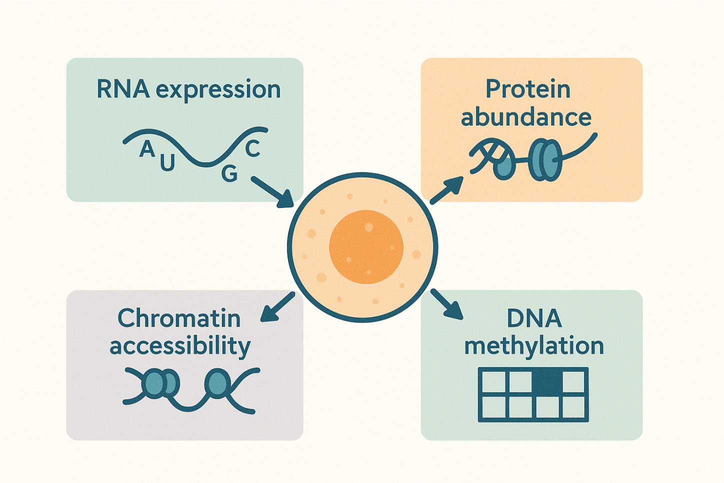
UChicago Statistics → Yale Statistics

Multimodal single-cell data



Each modality captures a different biological view

Multimodal data are ubiquitous

Examples with multiple high-dimensional data types

Field	**Object**	**Data types**
Computational biology	Tissue samples	Gene expression, microRNA, genotype, protein abundance/activity
Chemometrics	Chemicals	Mass spectra, NMR spectra, atomic composition
Atmospheric sciences	Locations	Temperature, humidity, particle concentrations over time
Internet traffic	Websites	Word frequencies, visitor demographics, linked pages

— from Lock et al. '13

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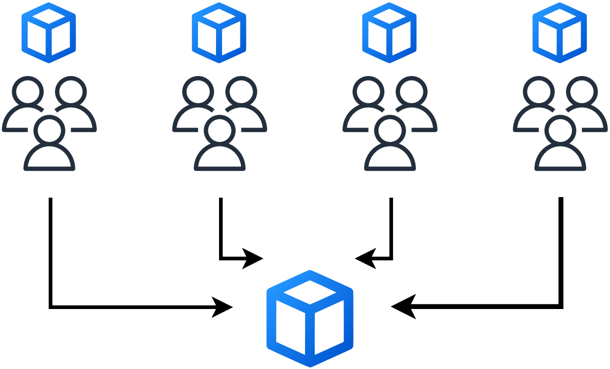
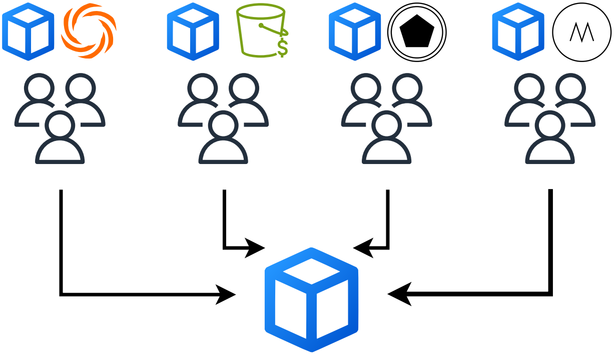
How to integrate information across different data types?

Learning shared structure



see e.g., Argelaguet et al. '18, Fan el al. '19, Arroyo et al. '22

Learning shared and unique structures



see e.g., Lock et al. '18, Lin and Zhang '23, Prothero et al. '24

Two key questions

- **Identification**: How to define shared and unique structures?
- **Estimation**: How to estimate shared and unique structures?

Joint and Individual Variation Explained (JIVE)

— Lock et el. '13

JIVE

We observe K matrices $\{\boldsymbol{A}_k\}_{1\leq k\leq K}$ with $\boldsymbol{A}_k \in \mathbb{R}^{n\times d_k}$ and

$$\boldsymbol{A}_k = \underbrace{\boldsymbol{U}^\star \boldsymbol{V}_k^{\star\top}}_{\substack{\text{rank}-r \\ \text{shared component}}} + \underbrace{\boldsymbol{U}_k^\star \boldsymbol{W}_k^{\star\top}}_{\substack{\text{rank}-r_k \\ \text{unique component}}} + \underbrace{\boldsymbol{E}_k}_{\text{Noise}}$$

- $\boldsymbol{U}^\star \in \mathbb{O}^{n\times r}$ is shared column space
- $\boldsymbol{U}_k^\star \in \mathbb{O}^{n\times r_k}$ are unique column spaces with $\boldsymbol{U}_k \perp \boldsymbol{U}$
- $\boldsymbol{V}_k^\star \in \mathbb{R}^{d_k\times r}$ and $\boldsymbol{W}_k^\star \in \mathbb{R}^{d_k\times r_k}$ are loading matrices

Two key questions

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Defining shared and unique structures in JIVE

JIVE

$$A_k^\star = \underbrace{U^\star V_k^{\star\top}}_{\substack{\text{rank}-r \\ \text{shared component}}} + \underbrace{U_k^\star W_k^{\star\top}}_{\substack{\text{rank}-r_k \\ \text{unique component}}}$$

JIVE defines shared information to be shared subspace $\cap_{k=1}^K \mathrm{col}(A_k^\star)$

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JIVE defines shared information to be shared subspace $\cap_{k=1}^K \mathrm{col}(\boldsymbol{A}_k^\star)$

But, does $\mathrm{col}(\boldsymbol{U}^\star) = \cap_{k=1}^K \mathrm{col}(\boldsymbol{A}_k^\star)$?

Faithfulness: $\mathrm{col}(\boldsymbol{U}^\star) \subset \cap_{k=1}^{K} \mathrm{col}(\boldsymbol{A}_k^\star)$

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- Counterexample: $\boldsymbol{V}_k^\star = \boldsymbol{W}_k^\star$
- Faithfulness is equivalent to assuming

$$\mathrm{rank}(\boldsymbol{A}_k^\star) = r + r_k$$

Exhaustiveness: $\cap_{k=1}^{K} \mathrm{col}(\boldsymbol{A}_k^\star) \subset \mathrm{col}(\boldsymbol{U}^\star)$

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Now, $\boldsymbol{U}^\star$ is identifiable since $\mathrm{col}(\boldsymbol{U}^\star) = \cap_{k=1}^{K} \mathrm{col}(\boldsymbol{A}_k^\star)$

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Angle-based JIVE (AJIVE)

— Feng et al. '18

AJIVE: a two-step spectral method

1. Estimate shared + unique column space of each $\boldsymbol{A}_k$:
   Let $\widetilde{\boldsymbol{U}}_k$ be top-$(r + r_k)$ left singular vectors of $\boldsymbol{A}_k$
2. Estimate shared column space:
   Let $\widehat{\boldsymbol{U}}$ be the top-r eigenvectors of $\sum_{k=1}^{K} \widetilde{\boldsymbol{U}}_k \widetilde{\boldsymbol{U}}_k^\top$

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$\leftarrow$ focus of this talk

Theoretical results

Key problem parameters

Performance of AJIVE and hardness of shared subspace estimation depend on

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— benefit of using multiple matrices?

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- K: number of matrices

  — benefit of using multiple matrices?
- θ: misalignment level of unique subspaces

Misalignment of unique subspaces

Recall for identifiability, we assume

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Definition 1 (Misalignment)

We say collection of subspaces $\{\boldsymbol{U}_k^\star\}_{1\le k\le K}$ is θ-misaligned if

$$\Bigg\| \frac{1}{K}\sum_{k=1}^{K} \boldsymbol{U}_k^\star \boldsymbol{U}_k^{\star\top} \Bigg\| \le 1-\theta$$

- θ tells us how misaligned unique subspaces are

Range of θ

θ-misalignment

$$\left\| \frac{1}{K} \sum_{k=1}^{K} \boldsymbol{U}_k^\star \boldsymbol{U}_k^{\star\top} \right\| \leq 1 - \theta$$

- Fully aligned: when $\cap_{k=1}^{K} \mathrm{col}(\boldsymbol{U}_k^\star) \neq \varnothing$, we have $\theta = 0$

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- Fully misaligned: when $\{\boldsymbol{U}_k^\star\}_{1 \leq k \leq K}$ are orthonormal to each other, we have $\theta = 1 - 1/K$
- Any $\theta \in (0, 1 - 1/K]$ is realizable by some $\{\boldsymbol{U}_k^\star\}$

Performance guarantees of AJIVE

Let $\sigma_{\min} := \min_k \sigma_{r+r_k}(\boldsymbol{A}_k)$

For simplicity suppose $n = d_1 = \cdots = d_K$, $r = r_1 = \cdots = r_K \asymp 1$

Theorem 2 (Yang, Ma '25)

Assume $\frac{\sigma\sqrt{n}}{\sigma_{\min}} \ll \min\{\sqrt{\theta}, \sqrt{K}\theta\}$. *AJIVE obeys*

$$\left\| \widehat{\boldsymbol{U}}\widehat{\boldsymbol{U}}^\top - \boldsymbol{U}^\star \boldsymbol{U}^{\star\top} \right\| \lesssim \frac{\sigma}{\sigma_{\min}} \sqrt{\frac{n}{K} + \frac{r}{K\theta}} + \frac{1}{\theta(1 \wedge K\theta)} \cdot \frac{\sigma^2 n}{\sigma_{\min}^2}$$

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- $\frac{\sigma}{\sigma_{\min}}\sqrt{\frac{n}{K} + \frac{r}{K\theta}}$: first-order error in high-SNR regime
- $\frac{1}{\theta(1 \wedge K\theta)} \cdot \frac{\sigma^2 n}{\sigma_{\min}^2}$: second-order error in low-SNR regime

High-SNR regime

Minimax lower bounds for estimating $\mathrm{col}(\boldsymbol{U}^\star)$

Theorem 3 (Yang, Ma '25)

$$\inf_{\widetilde{\boldsymbol{U}}} \sup_{\{\boldsymbol{A}_k^\star\}} \mathbb{E}\left[\left\|\widetilde{\boldsymbol{U}}\widetilde{\boldsymbol{U}}^\top - \boldsymbol{U}^\star\boldsymbol{U}^{\star\top}\right\|\right] \gtrsim \frac{\sigma}{\sigma_{\min}}\sqrt{\frac{n}{K} + \frac{r}{K\theta}}$$

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Recall upper bound of AJIVE when SNR is high:

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AJIVE is minimax optimal in high-SNR regime

Understanding optimal rate under high SNR

JIVE

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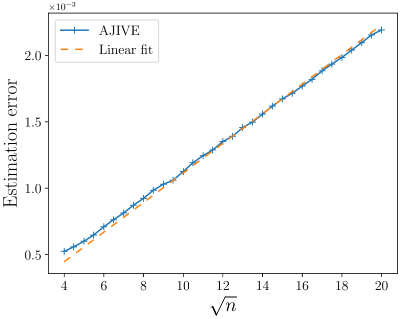
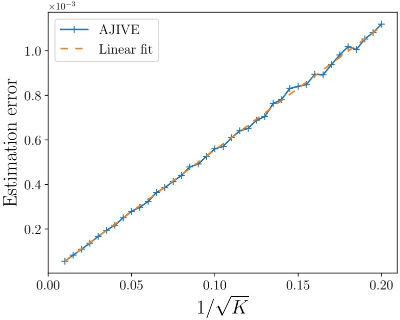
Shared subspace estimation is harder as unique subspaces are more aligned, i.e., θ is smaller

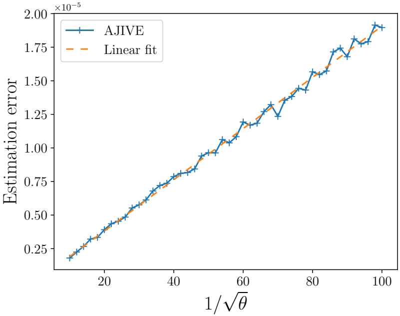
Empirical results: Large θ

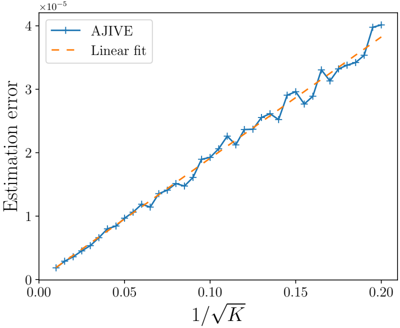




$$\theta = 0.5: \quad \|\widehat{\boldsymbol{U}\boldsymbol{U}}^\top - \boldsymbol{U}^\star \boldsymbol{U}^{\star\top}\| \propto \sqrt{n/K}$$

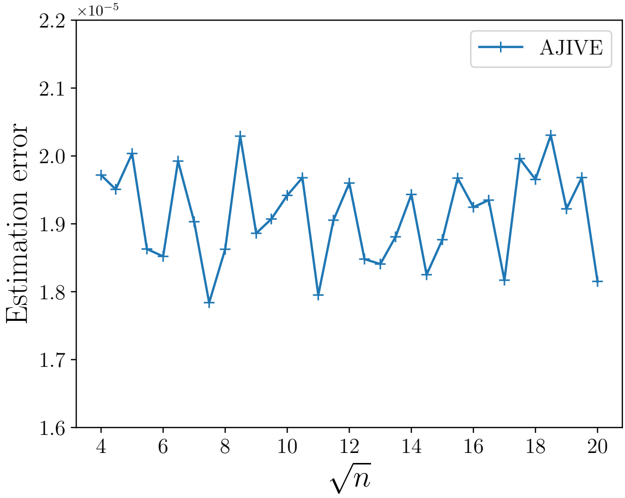
Empirical results: Small θ





$$\theta \in (0.0001, 0.01): \quad \|\widehat{\boldsymbol{U}}\widehat{\boldsymbol{U}}^\top - \boldsymbol{U}^\star \boldsymbol{U}^{\star\top}\| \propto \sqrt{1/K\theta}$$

Empirical results: Small θ



$$\theta = 0.0001$$

Low-SNR regime

Non-diminishing error in low-SNR regime

Revisiting upper bound of AJIVE when SNR is low:

$$\left\| \widehat{\boldsymbol{U}}\widehat{\boldsymbol{U}}^\top - \boldsymbol{U}^\star \boldsymbol{U}^{\star\top} \right\| \lesssim \frac{1}{\theta(1 \wedge K\theta)} \cdot \frac{\sigma^2 n}{\sigma_{\min}^2}$$

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Is this artifact in analysis or fundamental limitation?

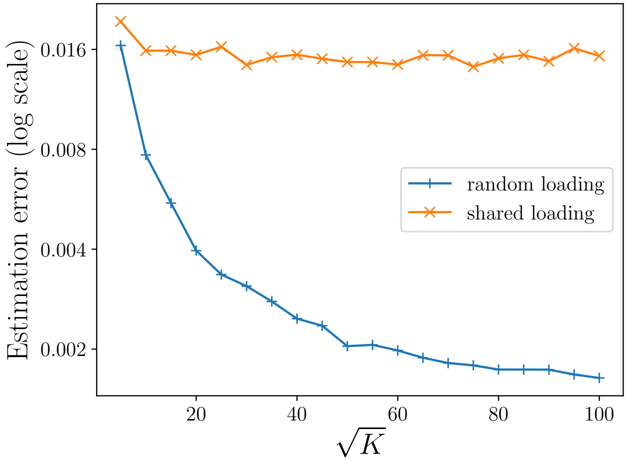
Two experimental settings

JIVE

$$\boldsymbol{A}_k = \underbrace{\boldsymbol{U}^\star \boldsymbol{V}_k^{\star\top}}_{\substack{\text{rank}-r \\ \text{shared component}}} + \underbrace{\boldsymbol{U}_k^\star \boldsymbol{W}_k^{\star\top}}_{\substack{\text{rank}-r_k \\ \text{unique component}}} + \underbrace{\boldsymbol{E}_k}_{\text{Noise}}$$

- Random loadings: $\boldsymbol{V}_k^\star$ and $\boldsymbol{W}_k^\star$ are independent random orthonormal matrices
- Shared loadings: Let $\boldsymbol{V}^\star$ and $\boldsymbol{W}^\star$ be random orthonormal matrices. Set $\boldsymbol{V}_k^\star = \boldsymbol{V}^\star$ and $\boldsymbol{W}_k^\star = \boldsymbol{W}^\star$ for all k

AJIVE has non-diminishing error



Shared vs random loadings on $\|\widehat{\boldsymbol{U}}\widehat{\boldsymbol{U}}^\top - \boldsymbol{U}^\star\boldsymbol{U}^{\star\top}\|$ vs K

Intuition: Bias aligns

AJIVE

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2. Let $\widehat{\boldsymbol{U}}$ be top-r eigenvectors of $\sum_{k=1}^{K} \widetilde{\boldsymbol{U}}_k \widetilde{\boldsymbol{U}}_k^\top$

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Is non-diminishing error fundamental to shared subspace estimation?

Oracle lower bound

Oracle spectral estimator

- Suppose unique components $\boldsymbol{U}_k^\star \boldsymbol{W}_k^{\star\top}$ are known, optimal estimator is top-r eigenspace of

$$\frac{1}{K}\sum_{k=1}^{K}\left(\boldsymbol{A}_k - \boldsymbol{U}_k^\star \boldsymbol{W}_k^{\star\top}\right)\left(\boldsymbol{A}_k - \boldsymbol{U}_k^\star \boldsymbol{W}_k^{\star\top}\right)^\top$$

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  For instance, oracle-aided estimate

$$\text{top-}r_k \text{ SVD of} \quad \mathcal{P}_\star^\perp \boldsymbol{A}_k = \boldsymbol{U}_k^\star \boldsymbol{W}_k^{\star\top} + \mathcal{P}_\star^\perp \boldsymbol{E}_k,$$

  where $\mathcal{P}_\star^\perp := \boldsymbol{I} - \boldsymbol{U}^\star \boldsymbol{U}^{\star\top}$

Non-diminishing error of oracle estimator

Oracle spectral estimator

1. Let $\widehat{\boldsymbol{U}}_k \widehat{\boldsymbol{W}}_k^\top$ be top-r_k SVD of $\mathcal{P}_\star^\perp \boldsymbol{A}_k = \boldsymbol{U}_k^\star \boldsymbol{W}_k^{\star\top} + \mathcal{P}_\star^\perp \boldsymbol{E}_k$
2. Let $\widehat{\boldsymbol{U}}_{\text{oracle}}$ be top-r eigenspace of

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Non-diminishing error of oracle estimator

Oracle spectral estimator

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Theorem 4 (Yang, Ma '25)

There exist $\boldsymbol{U}^\star$, $\{\boldsymbol{U}_k^\star\}_{k=1}^K$, $\{\boldsymbol{V}_k^\star\}_{k=1}^K$, $\{\boldsymbol{W}_k^\star\}_{k=1}^K$ *such that*

$$\left\|\widehat{\boldsymbol{U}}_{\text{oracle}} \widehat{\boldsymbol{U}}_{\text{oracle}}^\top - \boldsymbol{U}^\star \boldsymbol{U}^{\star\top}\right\| \geq C_2 \frac{\sigma^4 n^2}{\sigma_{\min}^4} - C_3 \frac{\log n}{\sqrt{K}} \cdot \frac{\sigma\sqrt{n}}{\sigma_{\min}}$$

Connection to nonconvex MLE

Maximum likelihood estimator

$$\min_{\boldsymbol{U},\boldsymbol{U}_k,\boldsymbol{V}_k,\boldsymbol{W}_k} \quad \sum_{k=1}^{K} \|\boldsymbol{U}\boldsymbol{V}_k^\top + \boldsymbol{U}_k\boldsymbol{W}_k^\top - \boldsymbol{A}_k\|_{\mathrm{F}}^2$$

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MLE can be inconsistent for estimating structural parameters

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Neyman–Scott problem:

- Bias in estimating σ^2:

$$E(s_i^2) = \frac{\sigma^2}{2} \quad \text{(not equal to } \sigma^2\text{)}$$

- As $n \to \infty$, MLE is inconsistent

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Setup: Probability of correct response of subject i to item j:

$$P(Y_{ij} = 1) = \frac{\exp(\theta_i - \beta_j)}{1 + \exp(\theta_i - \beta_j)}, \quad \text{for } 1 \le i \le n, 1 \le j \le m$$

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Y. Yang, and C. Ma, "Random pairing MLE for estimation of item parameters in Rasch model," arXiv:2406.13989, 2024

Neyman-Scott's problem in our case

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Y. Yang, C. Ma, "Estimating shared subspace with AJIVE: the power and limitation of multiple data matrices", arxiv:2501.093336, 2025