# Estimating Higher-Order Mixed Memberships via the $\ell_{2,\infty}$ Tensor Perturbation Bound

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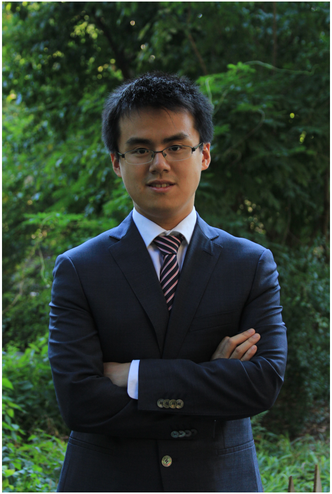
# Joint Work With:



Anru Zhang (Duke)

# Outline

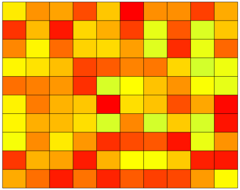
1. Motivation
2. Community Models
3. Estimation Algorithm
4. $\ell_{2,\infty}$ Tensor Perturbation
5. Data Analysis
6. Conclusion

# Outline

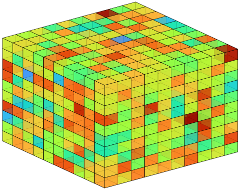
# Tensor Data

- A tensor is a multidimensional array.

Vector



Matrix



Order $3$ Tensor

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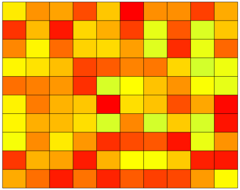

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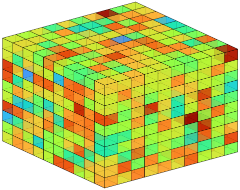

Order $3$ Tensor

- Can have higher-order tensors $\mathcal{T} \in \mathbb{R}^{p_1 \times \cdots \times p_d}$.
- This talk: focus on order $3$ tensors.

# Examples of Tensor Data

- Matrix time series

$$
\mathbf{M}_t = \begin{array}{l c}
 & \begin{array}{cccc} Apple & Twitter & Tesla & \cdots \end{array} \\
\begin{array}{l} Revenue_t \\ Assets_t \\ Dividends\ per\ share_t \\ \vdots \end{array} &
\begin{pmatrix}
X_{11}^{(t)} & X_{12}^{(t)} & X_{13}^{(t)} & \cdots \\
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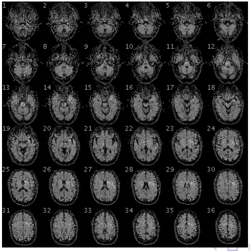
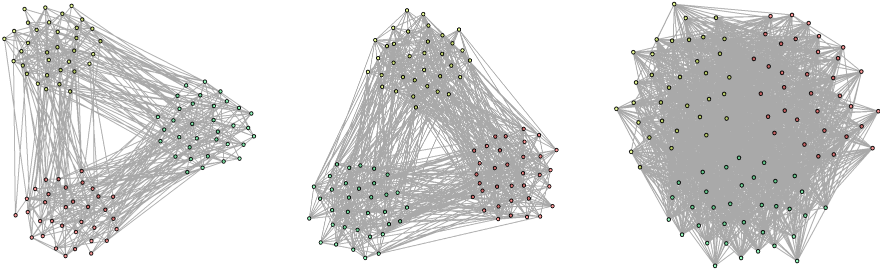
- Brain imaging data



# Special Case: Multilayer Networks

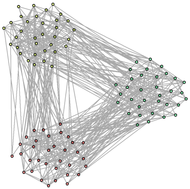
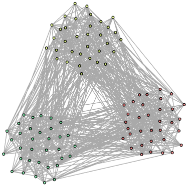
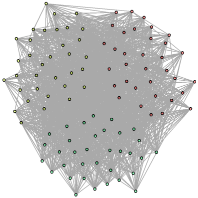
## Setting

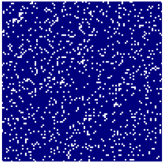
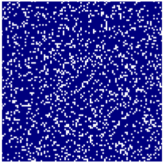
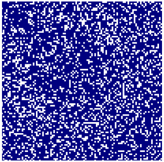
Observe $L$ networks on same $n$ vertices



# Multilayer Networks

Identify each network with its adjacency matrix:

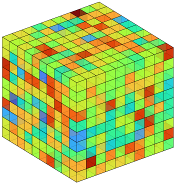




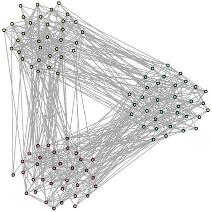
Organize adjacency matrices into $n \times n \times L$ Tensor!

# This Talk

**Main Question**

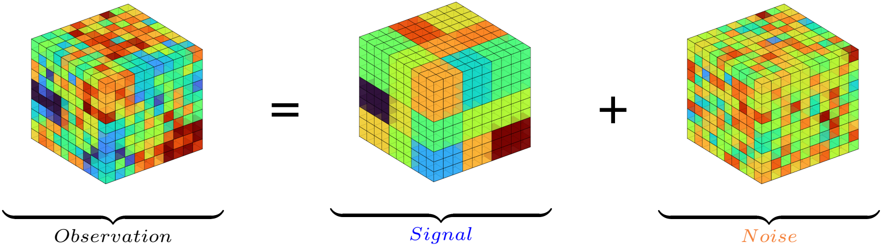
Given a noisy high-dimensional $p_1 \times p_2 \times p_3$ tensor with underlying community structure, can we consistently estimate the communities in the high dimensional regime $p_1, p_2, p_3 \asymp p$ as $p \to \infty$?





# Outline

# Tensor Blockmodels



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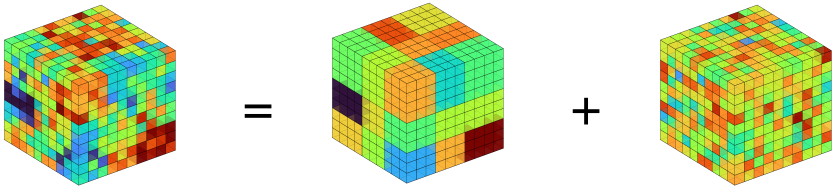

$$\underbrace{\mathit{Observation}} = \underbrace{\color{blue}{\mathit{Signal}}} + \underbrace{\color{orange}{\mathit{Noise}}}$$

## Interpretation

- There are $r_k$ communities *for each mode* ($k = 1, 2, 3$), and each node belongs to one community.
- Entry $i_1, i_2, i_3$ of the signal tensor is determined by community memberships of nodes $i_1$, $i_2$, and $i_3$.

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- Multilayer network with airports, airports, and airlines as the modes.

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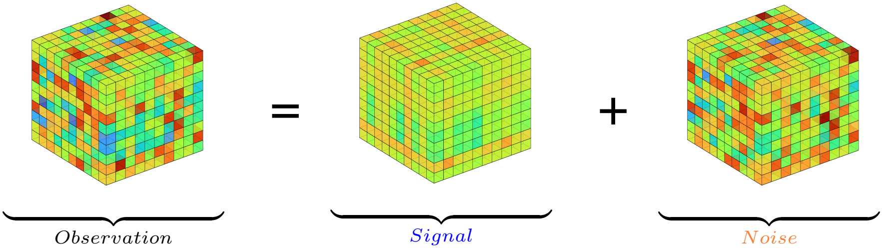
# Tensor Mixed-Membership Blockmodels



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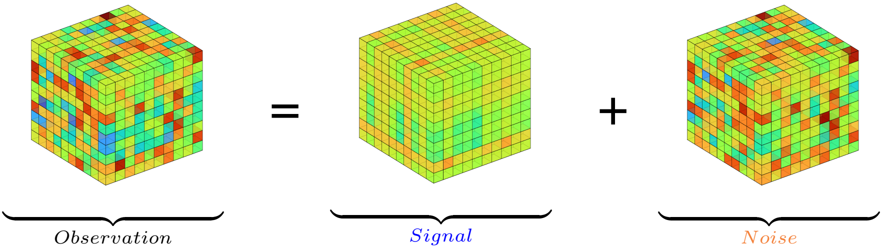

$$\underbrace{\text{(cube)}}_{Observation} = \underbrace{\text{(cube)}}_{Signal} + \underbrace{\text{(cube)}}_{Noise}$$

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- There are $r_k$ communities *for each mode* and each node belongs to *a convex combination of communities*.
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$$\mathcal{T}_{i_1 i_2 i_3} = \sum_{l_1=1}^{r_1} \sum_{l_2=1}^{r_2} \sum_{l_3=1}^{r_3} \mathcal{S}_{l_1 l_2 l_3} \left(\mathbf{\Pi}_1\right)_{i_1 l_1} \left(\mathbf{\Pi}_2\right)_{i_2 l_2} \left(\mathbf{\Pi}_3\right)_{i_3 l_3} \quad 1 \leq i_k \leq p_k;$$

$$\mathcal{T} = \mathcal{S} \times_1 \mathbf{\Pi}_1 \times_2 \mathbf{\Pi}_2 \times_3 \mathbf{\Pi}_3;$$

$\mathcal{S} \in \mathbb{R}^{r_1 \times r_2 \times r_3}$ is a $Mean\ Tensor$;

$\mathbf{\Pi}_k \in [0,1]^{p_k \times r_k}$ are $Mixed-Membership\ Matrices$ $(\|\left(\mathbf{\Pi}_k\right)_{i\cdot}\|_1 = 1)$

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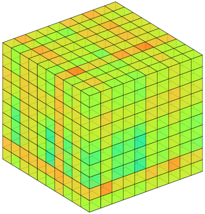
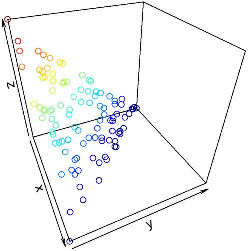


Underlying Tensor $\mathcal{T} \in \mathbb{R}^{p_1 \times p_2 \times p_3}$.

Extract $\mathbf{\Pi}_1$




$p_1$ Rows of matrix $\mathbf{\Pi}_1$.

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*Suppose each mode contains at least one pure node for each community and $\mathcal{S}$ is full rank. Then the model is identifiable up to community relabeling.*

Full rank: $\mathcal{S}$ can be written as matrix in three different ways – each of these is full rank.

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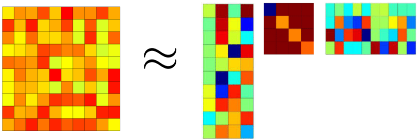
**Goal**

Estimate community membership matrices $\mathbf{\Pi}_1, \mathbf{\Pi}_2$, and $\mathbf{\Pi}_3 \in [0,1]^{p_k \times r_k}$.

# Outline

# Brief Detour: Tucker Decompositions and Tensor SVD

- Matrix SVD:



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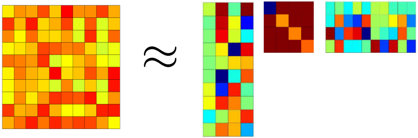

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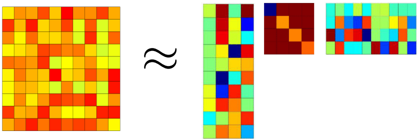
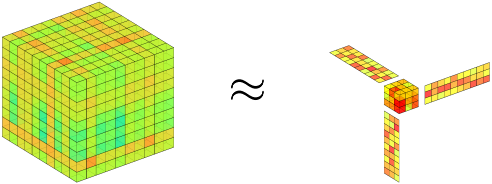


- No unified notion of Tensor SVD!
- Tensor mixed-membership blockmodel is related to Tucker decomposition



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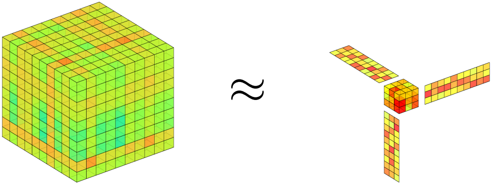

## Definition

A tensor $\mathcal{T}$ is rank $\mathbf{r} = (r_1, r_2, r_3)$ if $\mathbf{r}$ is the smallest triplet such that

$$\mathcal{T} = \mathcal{C} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \mathbf{U}_3;$$

$\mathcal{C} \in \mathbb{R}^{r_1 \times r_2 \times r_3}$ is a *core tensor*;

$\mathbf{U}_k \in \mathbb{R}^{p_k \times r_k}$ are orthonormal *loading matrices*.

Note: generalizes matrix SVD to higher-order.

# Spectral Geometry

**Proposition**

*Suppose* $\mathcal{T} = \mathcal{S} \times_1 \mathbf{\Pi}_1 \times_2 \mathbf{\Pi}_2 \times_3 \mathbf{\Pi}_3$ *is a tensor MMBM such that* $\mathcal{S}$ *is full rank with a pure node for each community along each mode. Let* $\mathcal{T} = \mathcal{C} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_2 \times_3 \mathbf{U}_3$ *be the rank* $(r_1, r_2, r_3)$ *Tucker factorization. Then*

$$\mathbf{U}_k = \mathbf{\Pi}_k \mathbf{U}_k^{(\mathrm{pure})},$$

*where* $\mathbf{U}_k^{(\mathrm{pure})} \in \mathbb{R}^{r_k \times r_k}$ *consists of the rows of* $\mathbf{U}_k$ *corresponding to pure nodes for mode* $k$*.*

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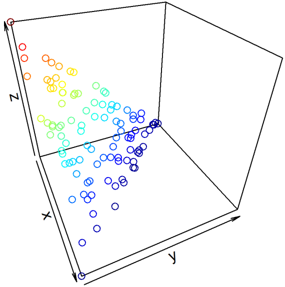
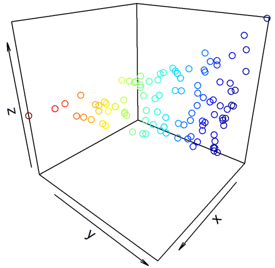



Rows of matrix $\mathbf{\Pi}_1$.

$$\xrightarrow{\mathbf{U}_1^{(\mathrm{pure})}}$$




Rows of loading matrix $\mathbf{U}_1$.

# Estimation Procedure

## Key Idea

Given an observation $\widehat{\mathcal{T}} = \mathcal{T} + \textrm{Noise}$:

1. First estimate the loading matrices $\mathbf{U}_1, \mathbf{U}_2$, and $\mathbf{U}_3$.
2. Next estimate pure nodes by finding the corners of the simplex associated to rows of $\mathbf{U}_k$ (standard corner-finding algorithms exist)
3. Estimate $\mathbf{\Pi}_k$ via plug-in from the equation $\mathbf{\Pi}_k = \mathbf{U}_k \big(\mathbf{U}_k^{(\mathrm{pure})}\big)^{-1}$.

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## Key Idea

Given an observation $\widehat{\mathcal{T}} = \mathcal{T} + \text{Noise}$:

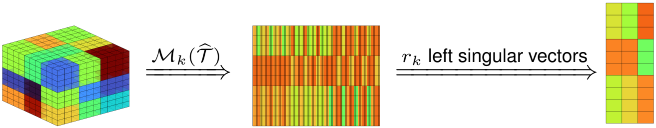
1. First estimate the loading matrices $\mathbf{U}_1, \mathbf{U}_2$, and $\mathbf{U}_3$.
2. Next estimate pure nodes by finding the corners of the simplex associated to rows of $\mathbf{U}_k$ (standard corner-finding algorithms exist)
3. Estimate $\mathbf{\Pi}_k$ via plug-in from the equation $\mathbf{\Pi}_k = \mathbf{U}_k \big(\mathbf{U}_k^{(\text{pure})}\big)^{-1}$.

## Problem

Need to estimate the loading matrices!

# Higher-Order SVD

- First straightforward guess: use leading $r_k$ left singular vectors of $\mathcal{M}_k(\widehat{\mathcal{T}})$



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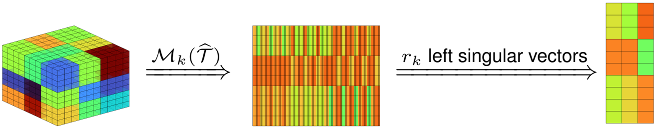


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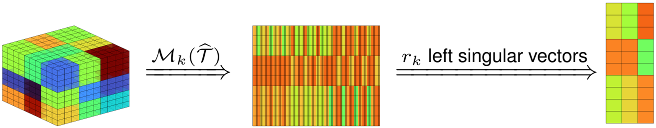


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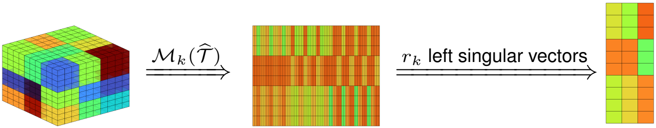


- Problem: can be suboptimal in high-noise regime!
- Why? Higher-Order SVD *ignores* tensor structure.

**Solution**

*Iteratively refine* the initial estimate using tensor structure!

# Higher-Order Orthogonal Iteration

- Given previous iterate $\widehat{\mathbf{U}}_k^{(t-1)}$ update $\widehat{\mathbf{U}}_k^{(t)}$ via

$$\widehat{\mathbf{U}}_1^{(t)} = r_1 \text{ left singular vectors of } \mathcal{M}_1\big(\widehat{\mathcal{T}} \times_2 \widehat{\mathbf{U}}_2^{(t-1)} \times_3 \widehat{\mathbf{U}}_3^{(t-1)}\big);$$

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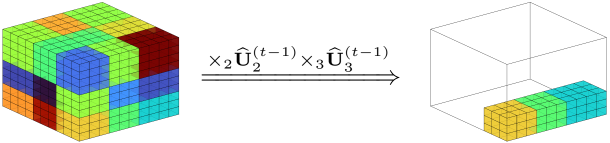

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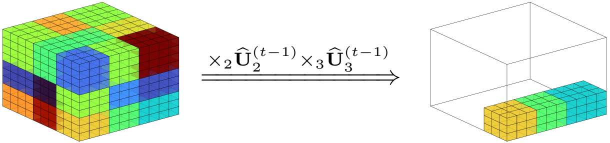


- Warm start: use modified spectral initialization to account for heteroskedastic noise.

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$$\widehat{\mathbf{\Pi}}_k = \widehat{\mathbf{U}}_k (\widehat{\mathbf{U}}_k^{(\text{pure})})^{-1}.$$

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*Let $\widehat{\mathbf{\Pi}}_k \in [0,1]^{p_k \times r_k}$ denote the estimated memberships with $t \asymp \log\left(\frac{\kappa r^{3/2}}{(\Delta/\sigma)p^{1/2}}\right)$ iterations for HOOI. Then there exist permutation matrices $\{\mathcal{P}_k\}$ such that with probability at least $1 - p^{-10}$ it holds that*

$$\max_{1 \leq i \leq p_k} \left\| \left( \widehat{\mathbf{\Pi}}_k - \mathbf{\Pi}_k \mathcal{P}_k \right)_{i\cdot} \right\| \leq C \frac{\kappa r^{3/2} \sqrt{\log(p)}}{(\Delta/\sigma) p}.$$

# Comparison to Matrix Setting

- For matrix mixed-membership blockmodel, it was previously shown that

$$\max_i \left\| \left( \widehat{\mathbf{\Pi}}^{(\text{Matrix})} - \mathbf{\Pi}^{(\text{Matrix})} \mathcal{P} \right)_{i\cdot} \right\| = \widetilde{O}\left( \frac{1}{\text{SNR} \times \sqrt{p}} \right).$$

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**Key Takeaway**

Higher-order structures *improve* estimation guarantees relative to the matrix setting.

Note: higher-order SVD results in row-wise error $O(1)$.

# Outline

# Proof Idea

- Recall the bound:

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Need to show that *each row of* $\widehat{\mathbf{U}}_k$ is sufficiently close to $\mathbf{U}_k$ with high probability.

# Technical Tool: $\ell_{2,\infty}$ Perturbation Bound

**Theorem ( Agterberg and Zhang (2022))**

*Let $\mathcal{T}$ be a rank $(r_1, r_2, r_3)$ tensor with Tucker decomposition $\mathcal{T} = \mathcal{C} \times_1 \mathbf{U}_1 \times_2 \mathbf{U}_3 \times \mathbf{U}_3$. Suppose that*

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# Previous Bounds

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$\Longrightarrow$ Errors are *spread out* along each row!

Note: result also depends on *spread-outedness* of the tensor.

# Optimality

$\lambda/\sigma = \mathrm{SNR} \geq C\kappa p^{3/4}\sqrt{\log(p)}$ (Our Requirement)

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$\Longrightarrow$ Optimal *up to factors of the condition number* $\kappa$ *and logarithmic terms.*

$\Longrightarrow$ Tensor MMBM SNR condition is essentially optimal.

Note: $\lambda \approx \Delta \frac{p^{3/2}}{r^{3/2}}$

# Proof Strategy

- Want to analyze the $i$'th row of the random variable $\widehat{\mathbf{U}}_1^{(t)} - \mathbf{U}_1 \mathbf{W}_1^{(t)}$

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Introduce special *leave-one-out sequences* that:

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Proof tracks *three separate* leave-one-out sequences (one for each mode) and the true sequence simultaneously by leveraging independence between leave-one-out sequences and noise.

# Outline

1. Motivation
2. Community Models
3. Estimation Algorithm
4. $\ell_{2,\infty}$ Tensor Perturbation
5. **Data Analysis**
6. Conclusion

# Analyzing Flight Network Data

- Setting: observe time-series of counts of flights between US airports from January 2016-September 2021
- Results in a tensor $\widehat{\mathcal{T}} \in \mathbb{R}^{343 \times 343 \times 69}$ (airports $\times$ airports $\times$ months)

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- Report community membership intensities for each community associated to pure nodes.

# Analyzing Flight Network Data: Airport Mode

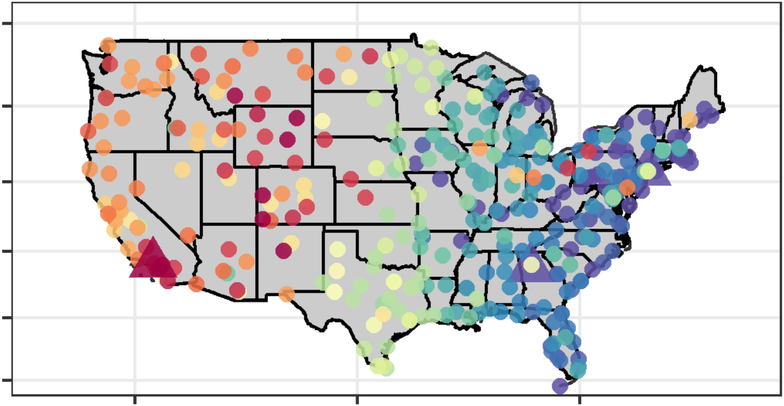

Figure: Community associated to the pure node LAX = Los Angeles. Red means higher membership intensity (closer to 1).

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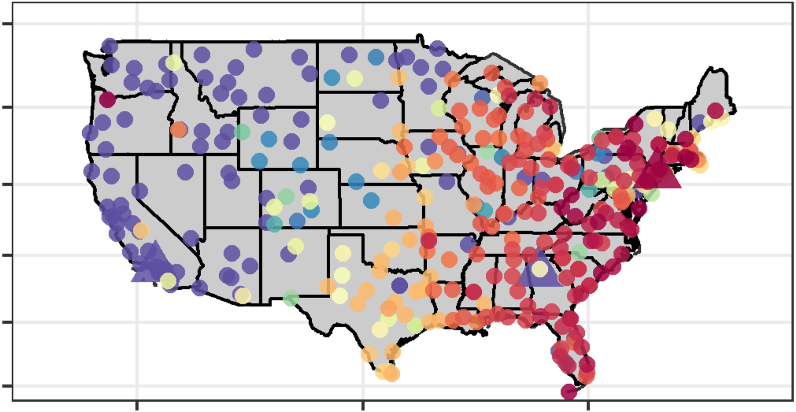

Figure: Community associated to the pure node LGA= New York. Red means higher membership intensity (closer to 1).

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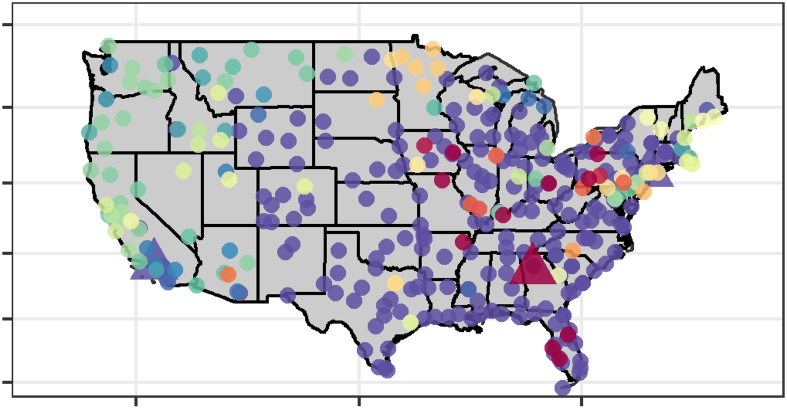
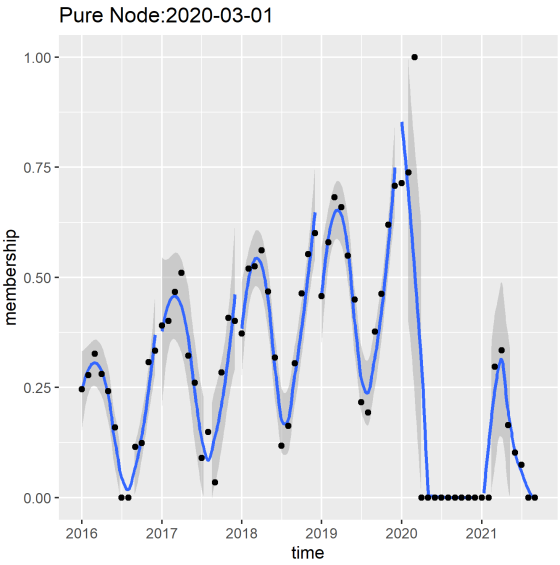


Figure: Community associated to the pure node ATL = Atlanta. Red means higher membership intensity (closer to 1).

# Analyzing Flight Network Data: Time Mode



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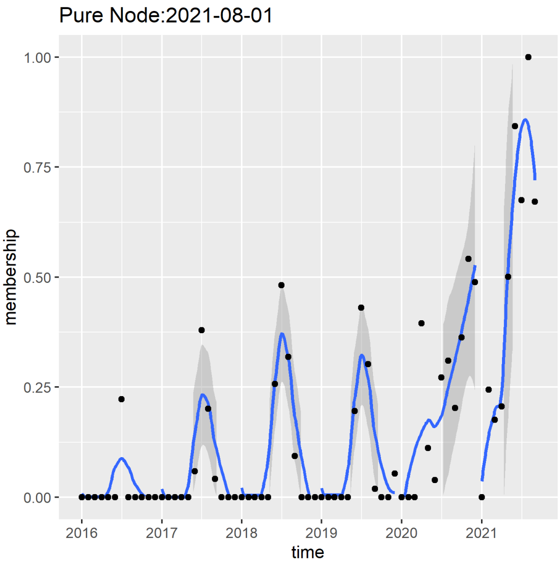

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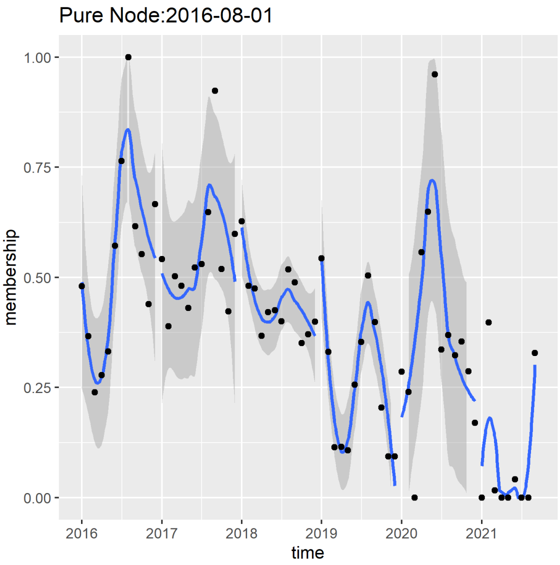

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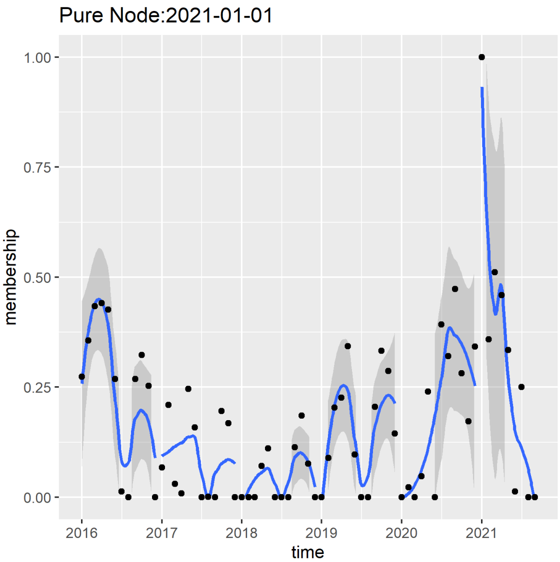

# Outline

# Conclusion

## Main Question

Given a noisy high-dimensional $p_1 \times p_2 \times p_3$ tensor with underlying community structure, can we consistently estimate the communities in the high dimensional regime $p_1, p_2, p_3 \asymp p$ as $p \to \infty$?

# Conclusion

## Main Question

Given a noisy high-dimensional $p_1 \times p_2 \times p_3$ tensor with underlying community structure, can we consistently estimate the communities in the high dimensional regime $p_1, p_2, p_3 \asymp p$ as $p \to \infty$?

## Answer

Yes! The maximum row-wise error rate yields an improvement of order $\sqrt{p}$ for a $p \times p \times p$ tensor relative to a $p \times p$ matrix!

# Future and Ongoing Work

- Multilayer networks:
  - Ameliorating degree heterogeneity (Agterberg et al., 2022)
  - More general community models with estimation and testing guarantees with multilayer networks
  - Estimation accuracy in sparse network regimes
  - Network time series

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  - Robustness and sparsity
- Spectral methods and nonconvex algorithms:
  - Entrywise guarantees for other nonconvex matrix and tensor algorithms under different noise models
  - Inference with the outputs of nonconvex procedures
  - Heterogeneous missingness mechanisms

# References I


Joshua Agterberg and Anru Zhang. Estimating Higher-Order Mixed Memberships via the $\ell_{2,\infty}$ Tensor Perturbation Bound, December 2022. arXiv:2212.08642 [math, stat].

Joshua Agterberg, Zachary Lubberts, and Jesús Arroyo. Joint Spectral Clustering in Multilayer Degree-Corrected Stochastic Blockmodels, December 2022. arXiv:2212.05053 [math, stat].

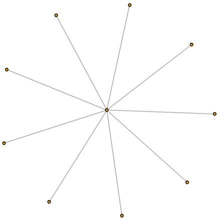
# Thank you!

: @JAgterberger

# Correcting For Hubs

## Observation

One community in the airport data was a *hub community*.



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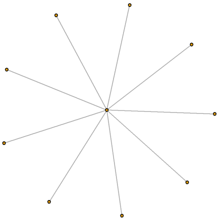
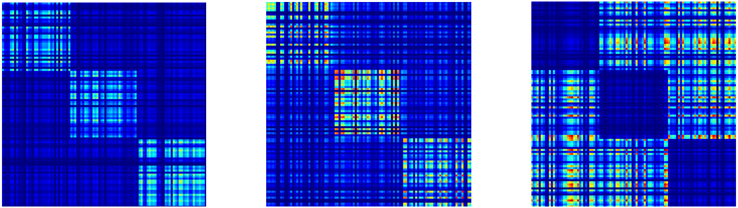


**Question**

Can we still obtain good estimation by *accounting for hubs in the model*?

# Multilayer Degree-Corrected Stochastic Blockmodel



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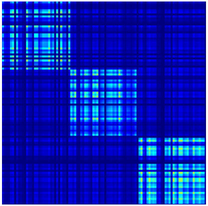

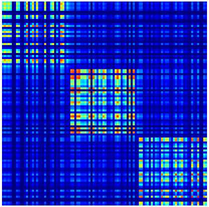

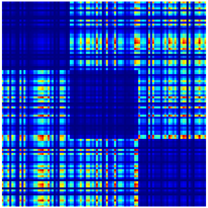

## Interpretation

Observe the *same communities* across the networks, but the means are different *and vertices are permitted to differ between and within networks*.

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- Each vertex $i$ belongs to community $z(i)$.

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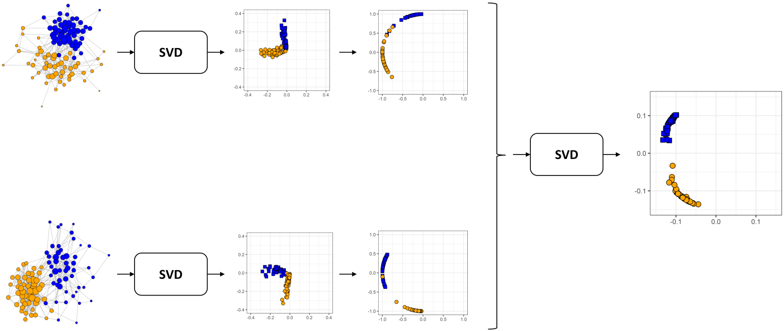
**Goal**

Use all $L$ networks to estimate community memberships.

# DC-MASE: Degree-Corrected Multiple Adjacency Spectral Embedding



# Theoretical Guarantees

**Theorem (Informal Restatement of Theorem 1 of Agterberg et al. (2022))**

*Consider a multilayer DCSBM with each network having* ***the same signal strength****, and suppose each edge probability matrix has rank* $K$*. Let* $\widehat{z}$ *denote the output of clustering with K-means on the rows of the output of DC-MASE, and define*

$$\ell(\widehat{z}, z) := \frac{\#\textit{misclustered nodes}}{n}.$$

*Then*

$$\mathbb{E}\ell(\widehat{z}, z) \leq \frac{2K}{n} \sum_{i=1}^{n} \exp\Bigg( - cL\theta_i \times (\mathrm{SNR}\textit{-like term})\Bigg).$$

Note: the same signal strength condition is not required in the main result.

Note: number of misclustered nodes is up to permutation of community labels.

# Improving Estimation?

- Has been demonstrated that vanilla spectral clustering (using a slightly different procedure) achieves the error rate:

$$\mathbb{E}\ell(\widehat{z}, z) \leq \frac{2K}{n}\sum_{i=1}^{n}\exp\Big(-c\theta_i \times (\mathrm{SNR}\text{-like term})\Big).$$

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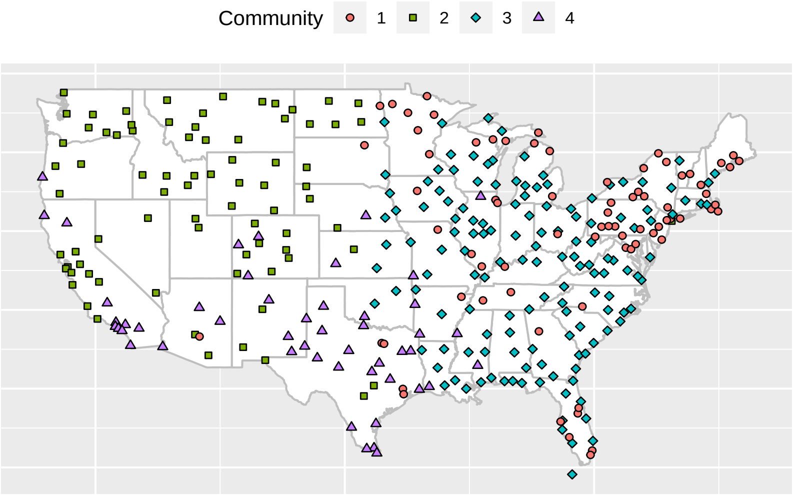
**Key Takeaway**

Multiple networks *improve* estimation guarantees (relative to the single network setting).

# Analyzing Flight Network Data



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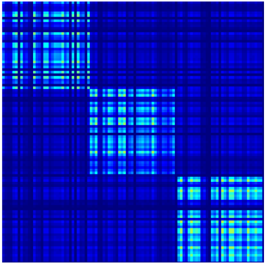
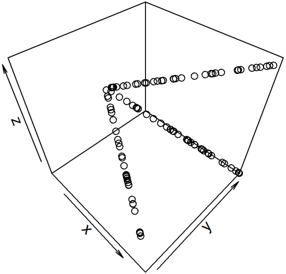
# Spectral Geometry

**Observation 1**

Each population network is rank $K$, with rows of scaled eigenvectors supported on one of $K$ rays, where $K$ is the number of communities.



Population adjacency matrix

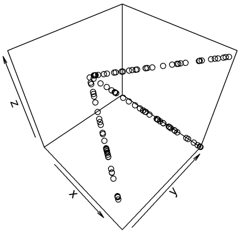



Rows of scaled eigenvectors of population adjacency matrix, viewed as points in dimension $K = 3$

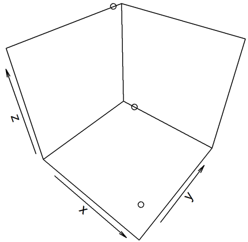
# Spectral Geometry

## Observation 2

Projecting each ray to the sphere results in community memberships for a single network.




Rows of scaled eigenvectors of population adjacency matrix, viewed as points in dimension $K = 3$



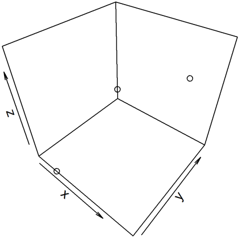

Row-normalized scaled eigenvectors of population adjacency matrix, viewed as points in dimension $K = 3$

# Spectral Geometry

**Observation 3**

$n \times LK$ matrix of concatenated row-normalized embedding has left singular subspace that reveals community memberships for all networks.

$n \times LK$ matrix of concatenated row-normalized embedding.




Rows of left singular vectors viewed as points in dimension $K = 3$