

# Multivariate Analysis of Large-Scale Network Series

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# Network Data

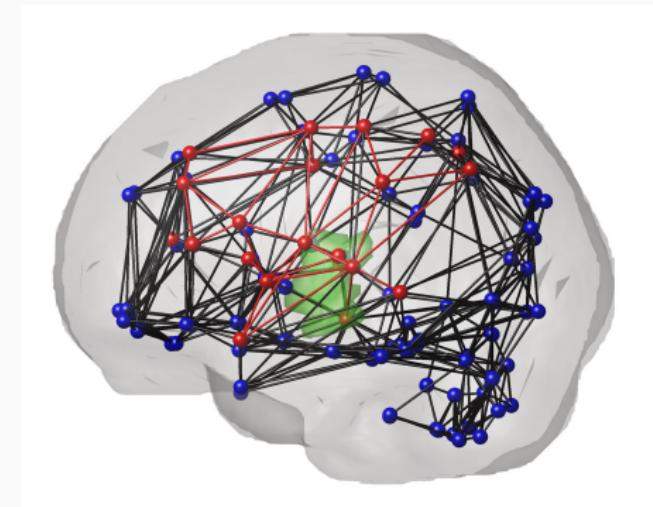
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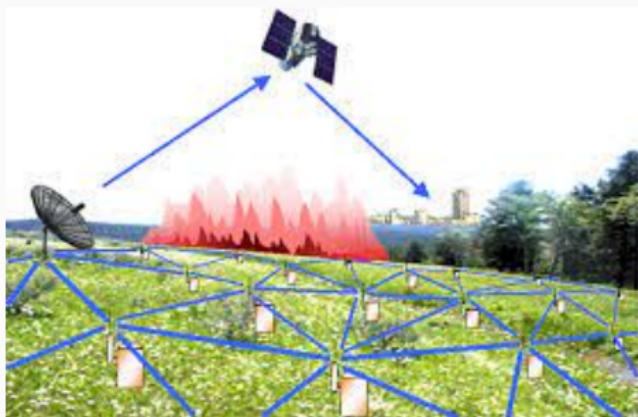


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Today: contributions to **network science** on multiple networks

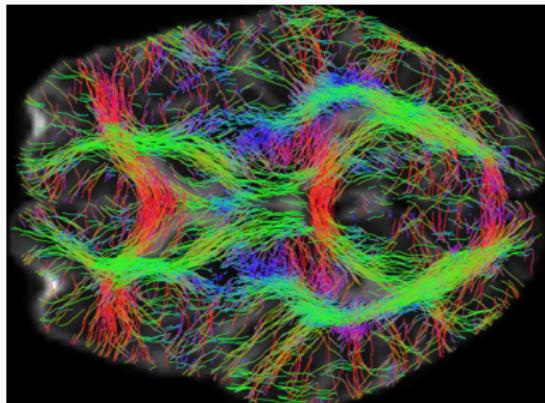
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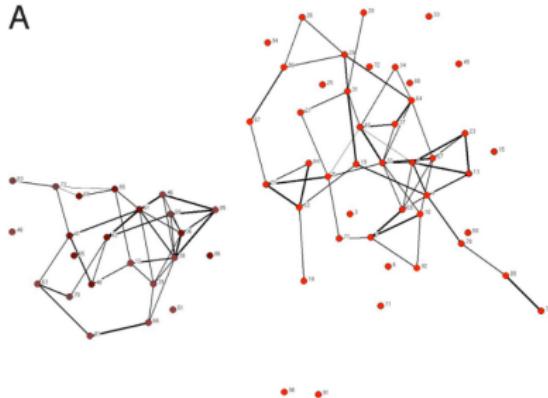


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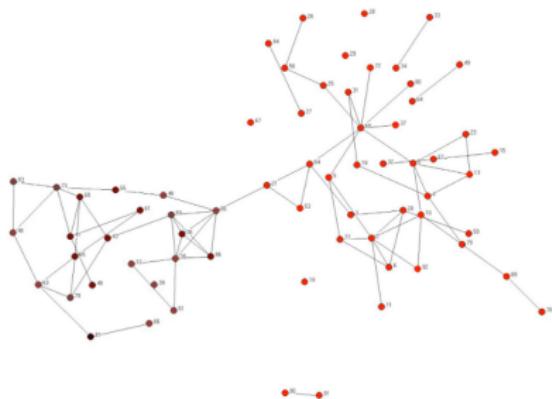
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A



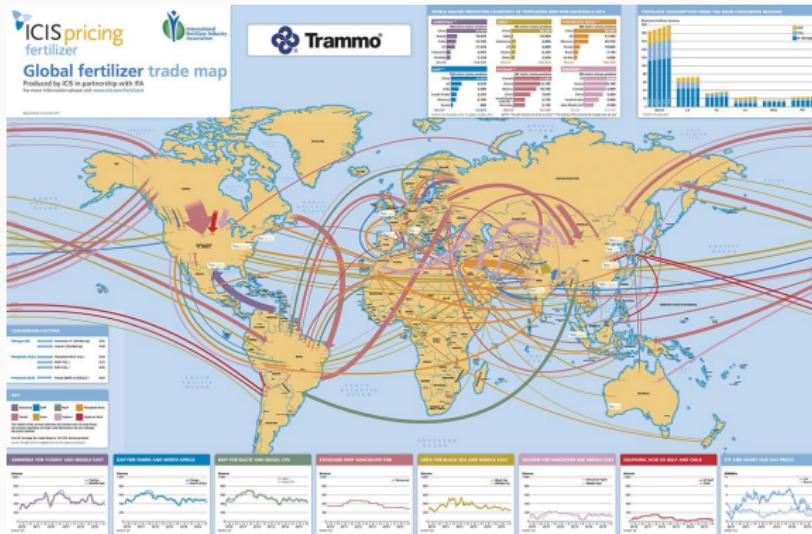
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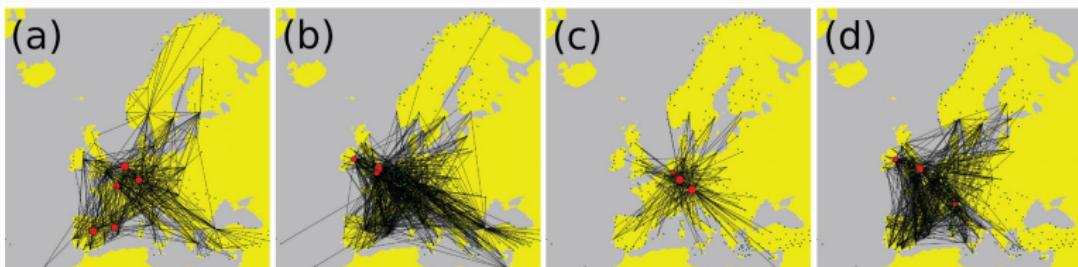
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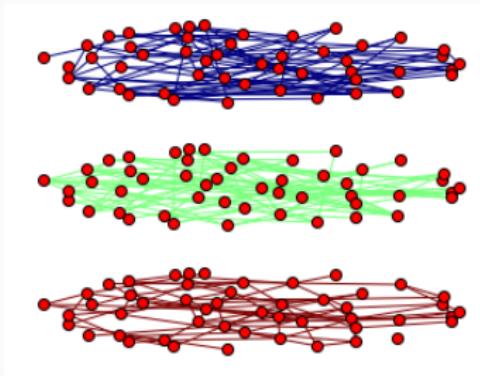
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Network Series: an ordered set of network observed on the same nodes

Special Case of “Multilayer Networks” (*Kivelä et al., J. Complex Networks, 2014*)

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Clustering:

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Joint Embeddings:

- Wang *et al.*, *PAMI*, 2021

# **Multivariate Methods for Multiple Networks**

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## Acknowledgements

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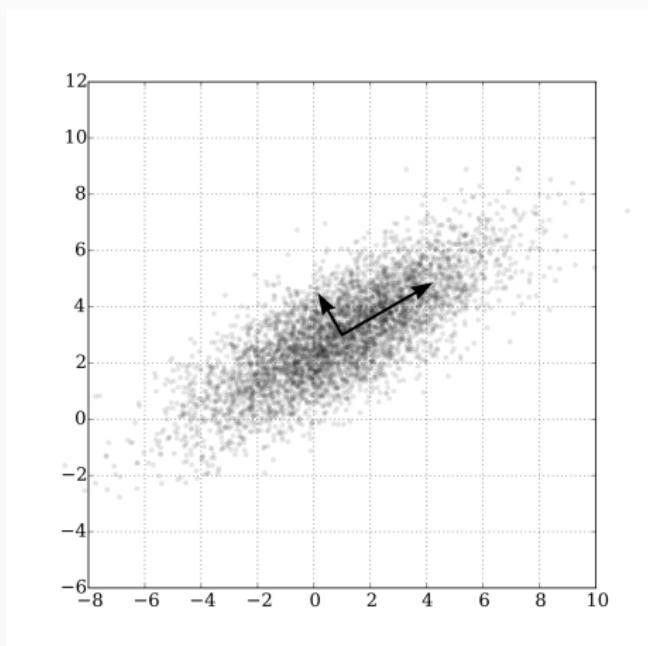
IC Advisors: Joe McCloskey (NCSC) + Steve H (GCHQ)



# Principal Components Analysis

## Principal Components Analysis:

- Exploratory Data Analysis
- Pattern Recognition
- Dimension Reduction
- Data Visualization



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Data matrix:  $X \in \mathbb{R}^{n \times p}$

- $n$  observations (rows)
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Decompose  $X$  into a **major pattern**  $\mathbf{v}$  and **how much the pattern contributes to each observation**  $\mathbf{u}$

All-purpose pattern recognition tool:

- Raw  $X$  - major patterns (trends)
- Centered  $X$  - variance components (covariance patterns)
- Differenced  $X$  - change-point identification (CUSUM analysis)

# Tensor Analysis

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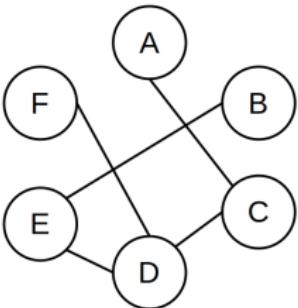
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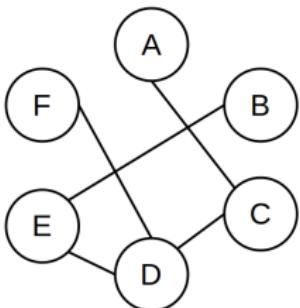


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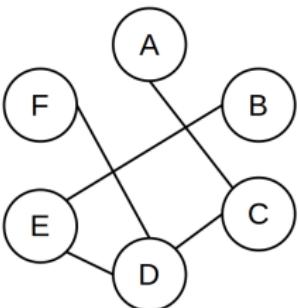
	A	B	C	D	E	F
A	0	0	1	0	0	0
B	0	0	0	0	1	0
C	1	0	0	1	1	0
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- Identify edges for each network
- Create a  $p \times p$  **adjacency matrix**
- Align into a  $p \times p \times T$  **tensor**



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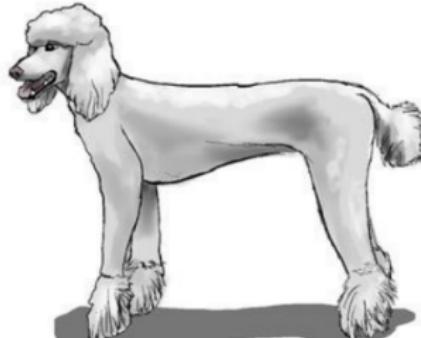
Scalar



Vector



Matrix



Tensor



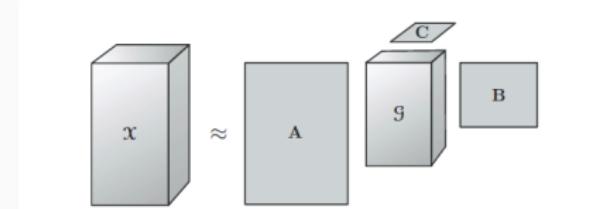
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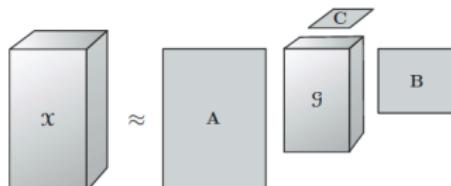
- Tucker Factors: Optimal for compression; limited interpretation



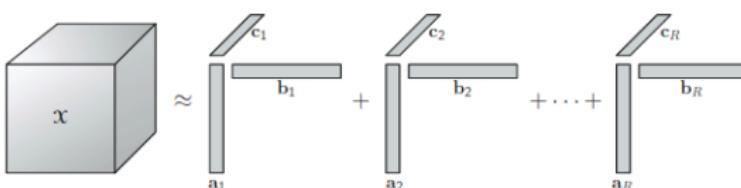
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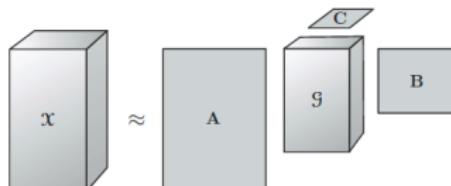


Regularized variants available (Allen, AISTATS, 2012)

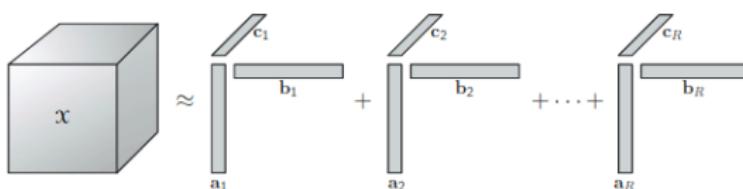
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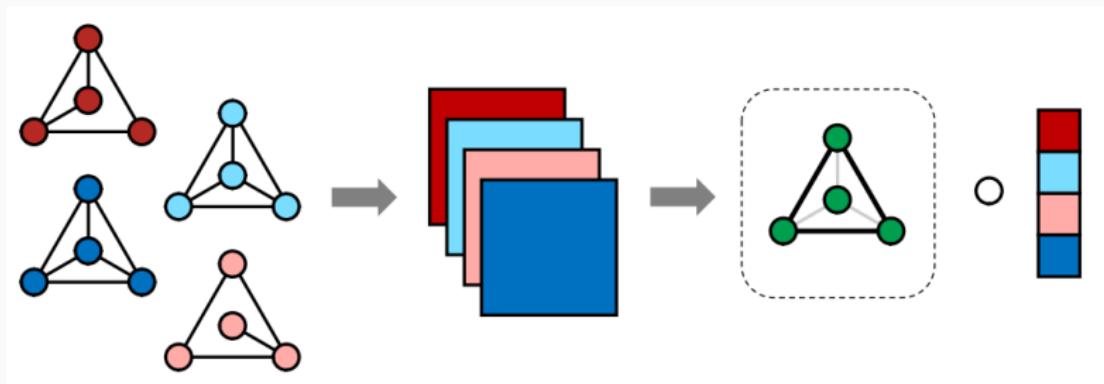
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Both well-studied: neither uses the network structure of our tensor

Semi-Symmetric Tensor Decomposition Needed

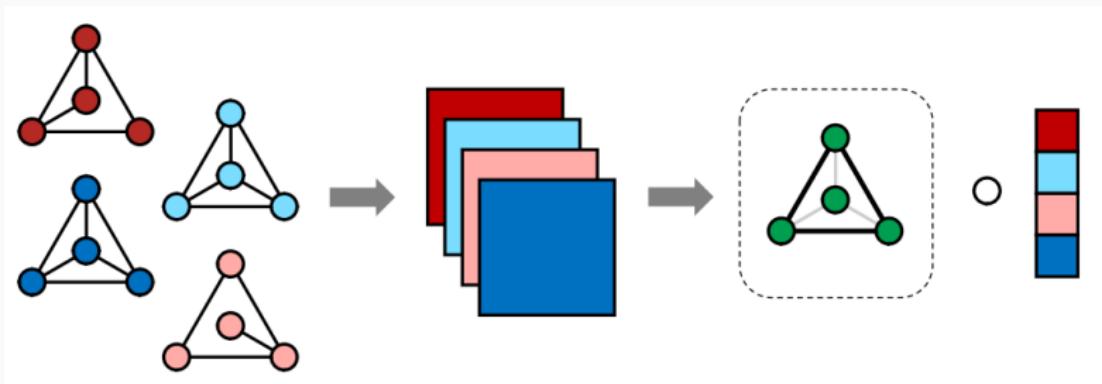
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Goals:

- Preserve Network Structure
- Computational AND Statistical Efficiency
- Flexibility - Capture Arbitrary Low-Rank Factors
- Nestability - Capture Multiple Principal Components

# Semi-Symmetric Tensor PCA

Semi-Symmetric Generalization of the CP decomposition:

$$\mathcal{X} \approx \sum_{i=1}^k d_i V_i \circ V_i \circ u_i$$

where  $V_i \in \mathbb{R}^{p \times r_i}$  is orthogonal,  $u_i \in \mathbb{R}^T$ .

$(r_1, \dots, r_k)$ -SS-TPCA

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Rank-1 model applied in multi-subject neuroimaging to find PC factors correlated with behavioral traits (Zhang et al., NeuroImage 2019)

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Alternating maximization approach:  $u$  and  $V$  subproblems are tractable!

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Disadvantages:

- Non-Convex
- Mildly Sensitive to Initialization

## Statistical Consistency

“Spiked Covariance / Low-Rank Mean” Model:

$$\mathcal{X} = d V_* \circ V_* \circ u_* + \mathcal{E}$$

Does the Semi-Symmetric Tensor Power Method recover  $u_*$  and  $V_*$ ?

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- Recovery up to orthogonal rotation

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### Applied Math:

- Sorensen and De Lathauwer, *SIMAX*, 2015
  - Considered our model as a  $(L_r, L_r, 1)$ -Multilinear Rank Decomposition
  - No “statistical” theory

# Statistical Consistency

## Theorem (Semi-Formal)

Suppose  $\mathcal{X} = d V_* \circ V_* \circ u_* + \mathcal{E}$  where

- $u_*$  is a unit-norm  $T$ -vector
- $V_*$  is a  $p \times r$  orthogonal matrix satisfying  $V_*^T V_* = I_{r \times r}$
- $d \in \mathbb{R}_{>0}$  is a measure of signal strength
- $\mathcal{E}$  is a semi-symmetric noise tensor each free element of which is independently  $\sigma$ -sub-Gaussian.

With sufficiently good iteration, our Algorithm applied to  $\mathcal{X}$  satisfies the following with high probability:

$$\min_{O \in \mathcal{V}^{k \times k}} \frac{\|V^* - \hat{V}O\|_2}{\sqrt{pr}} \lesssim \frac{\sigma r \sqrt{T}}{d} \quad \text{and} \quad \min_{\epsilon \in \{\pm 1\}} \frac{\|u^* - \hat{u}\epsilon\|_2}{\sqrt{T}} \lesssim \frac{\sigma r \sqrt{p}}{d}$$

Furthermore the statistical convergence is linear (fast) before hitting the “noise barrier”

## Proof Outline

Davis-Kahan theorem applied repeatedly + iteration:

V-update:

$$\|\sin \angle(V^*, V^{(k+1)})\|_F \leq 2 \left| 1 - \cos \angle(u^{(k+1)}, u_*) \right| + \frac{2 \|\mathcal{E}\|_{r\text{-op}}}{d}$$

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u-update:

$$|\sin \angle(u_*, u^{(k+1)})| \leq 2 \left| 1 - \cos \angle(V_*, V^{(k)})^4 \right| + \frac{4r \|\mathcal{E}\|_{r\text{-op}}}{d} + \frac{2r^2 \|\mathcal{E}\|_{r\text{-op}}^2}{d^2}$$

Surprisingly tricky deal with normalization of u updates

$\implies$  apply DK to  $\lambda \tilde{u}_k \circ \tilde{u}_k - u_* \circ u_*$  for suitable  $\lambda$

## Proof Outline

Davis-Kahan theorem applied repeatedly + iteration:

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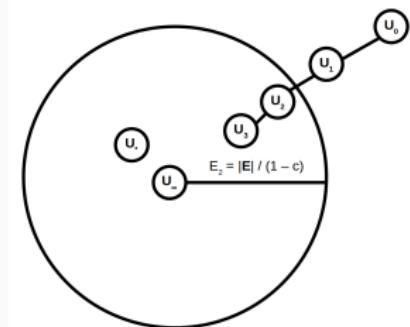
Chain + iterate to desired bound

# Convergence Rate

More detailed work shows that:

$$\text{Error at Iteration } k \approx c^k E_1 + E_2 / (1 - c)$$

where



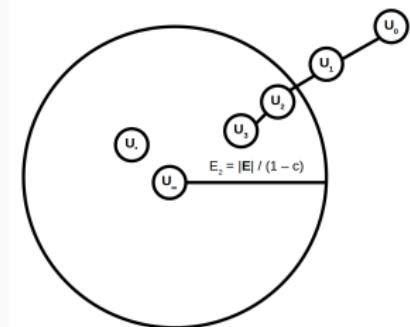
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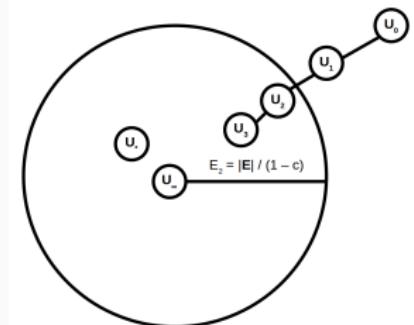
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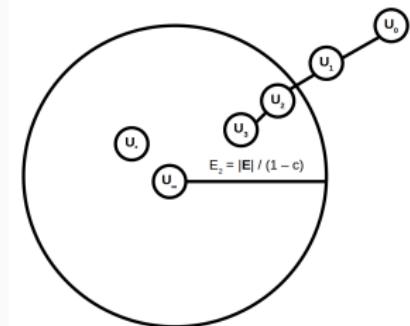
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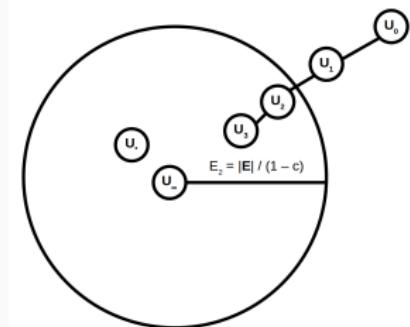
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Implications:

- Geometric convergence to “noise range”
- Possibly slow (or looping) after that

Similar results obtained for sparse regression by Fan *et al.* (AoS, 2018)

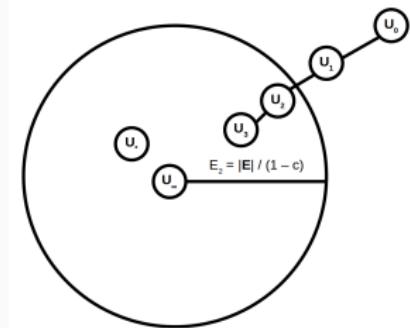
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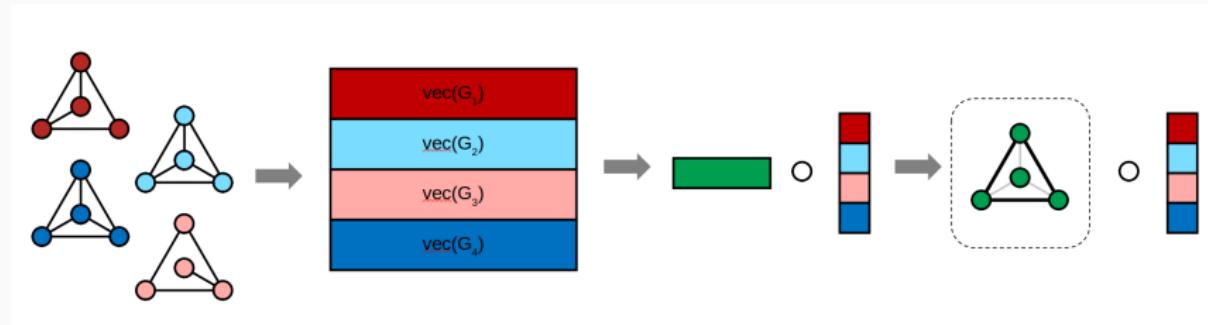
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All this despite non-convexity: analyze *algorithm* not *problem*!

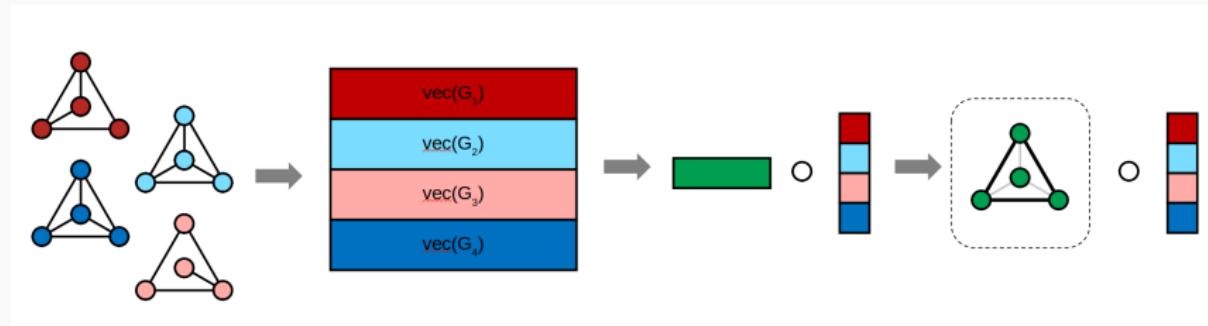
# Is this just PCA?

Weighted networks + (real) inner product - perform a spectral decomposition in this space (Eaton, 1983)?



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Does not enforce rank- $r$  structure on “principal network:” SS-TPCA is equivalent to

$$\arg \max_{u,v} u^T \mathcal{M}_3(\mathcal{X}) v \text{ such that } \text{rank}(\text{unvec}(v)) = r$$

Variant of Truncated Power Method for Sparse PCA (Yuan and Zhang, JMLR 2013) with “unvec-rank” instead of sparsity constraint

## Comparison with Classical PCA

Method	Dimension	$u$ -MSE	$v$ -MSE
Classical PCA	$T \times p$	$\frac{\sigma\sqrt{p}}{d}$	$\frac{\sigma\sqrt{T}}{d}$

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Tensor approach:

- Same rate as classical PCA (when  $r = 1$ )
- Better than naïve (vectorization) approach by factor of  $\sqrt{p} \gg r$

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Connection to “unvec-rank” constrained PCA highlights key role of Davis-Kahan in theoretical analysis

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# Practicalities

## Initialization:

- For many network problems, signal is roughly constant (or at least positive)
  - Stable initialization:  $u_0 = 1/\sqrt{T}$
  - Performs particularly well for trend-finding and change-point
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- Selecting  $r$  too high usually harmless

## Application: SCOTUS Voting

---







Can we use network analysis to identify voting  
patterns among SCOTUS Justices?

# SCOTUS Network Data

Each term SCOTUS decides  $\approx 80$  cases:

- Create a **weighted, undirected** network based on co-voting<sup>1</sup>
- Analyze by “seat” (AJ7 = Ginsburg = Barrett), not by Justice

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Data: SCOTUSblog annual “stat pack” - OT 1995 to OT 2020

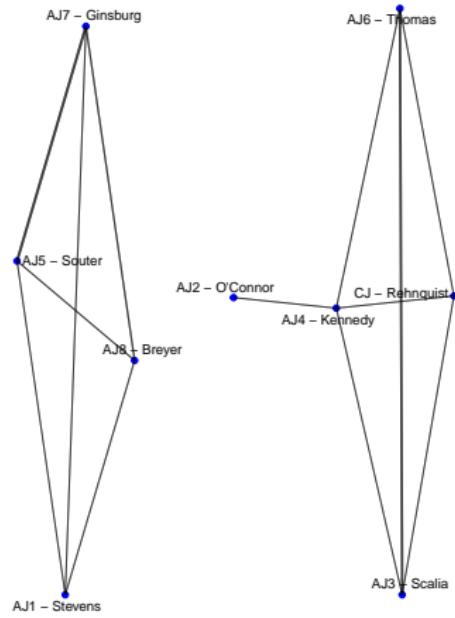
The screenshot shows the SCOTUSblog homepage. At the top, there's a banner featuring a painting of the Supreme Court building with flags. Below the banner is a navigation bar with links for #, CASES, PETITIONS, STATISTICS, NEWSFEED, CATEGORIES, ABOUT, and social media icons for Facebook, Twitter, and Instagram. A search bar is also present. The main content area has a heading "SCOTUS NEWS" and a prominent red banner with the text "Justices to hold in-person arguments in the fall". Below the banner, a smaller text says "By Amy Howe on Sept. 8 at 1:10 p.m." and a paragraph about the resumption of in-person arguments. To the right of the text is a photograph of the Supreme Court courtroom, showing red curtains and the bench.

$$9 \times 9 \text{ pairs} \times 25 \text{ terms} \equiv \mathcal{X} \in \mathbb{R}^{9 \times 9 \times 25}$$

<sup>1</sup>We consider agreement *in the judgement*, not in reasoning.

# Example - OT 2001

October Term 2001



# Semi-Symmetric PCA as a Flexible Pattern Recognition Tool

Semi-Symmetric PCA as a Flexible Pattern Recognition Tool:

- Raw  $\mathcal{X}$  - major patterns (trends)
- Centered  $\mathcal{X}$  - variance components (covariance patterns)
- Differenced  $\mathcal{X}$  - change-point identification (CUSUM analysis)

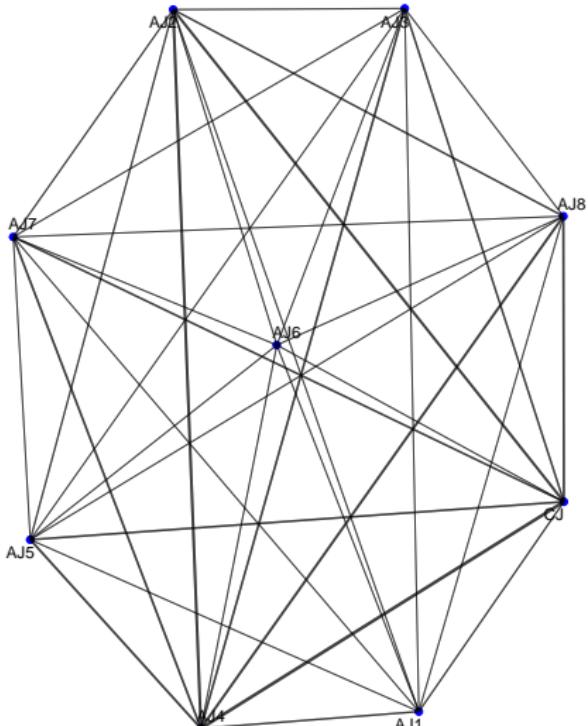
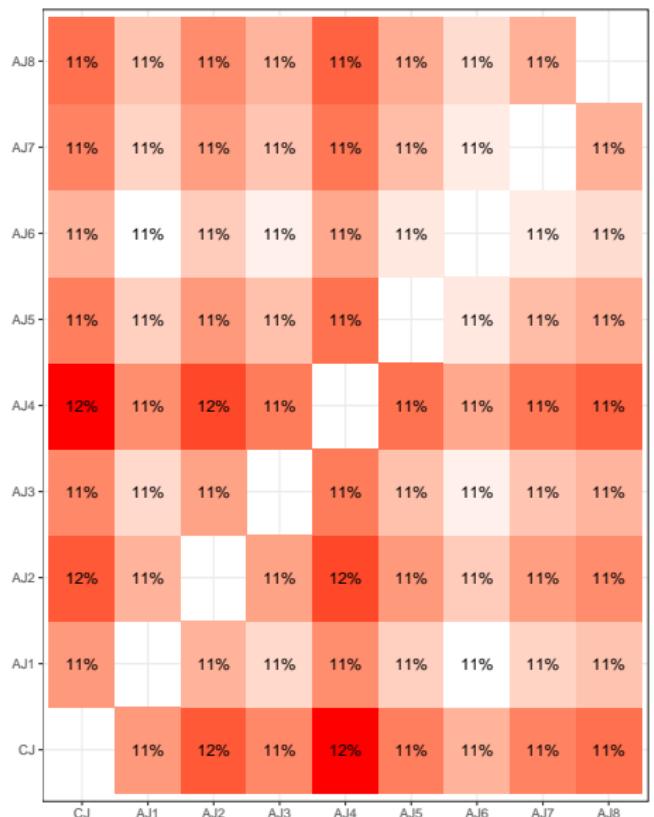
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# Baseline (Mean) Court Behavior

The majority of SCOTUS cases are decided (nearly) unanimously



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VIDEO

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CORONAVIRUS



## Supreme Court defies critics with wave of unanimous decisions

*Chief Justice John Roberts is credited with fostering consensus on high court.*

By **Devin Dwyer**

June 29, 2021, 4:12 AM • 11 min read



Sections

The Washington Post

*Democracy Dies in Darkness*

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# Those 5-to-4 decisions on the Supreme Court? 9 to 0 is far more common.

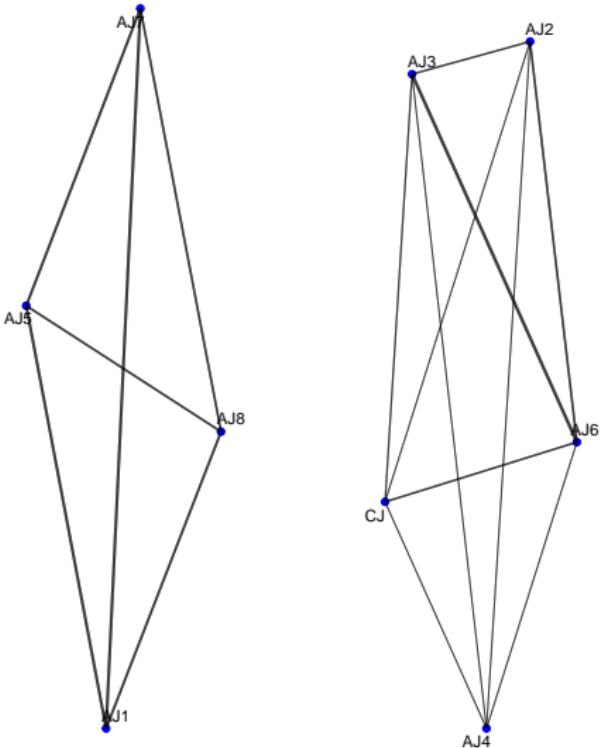
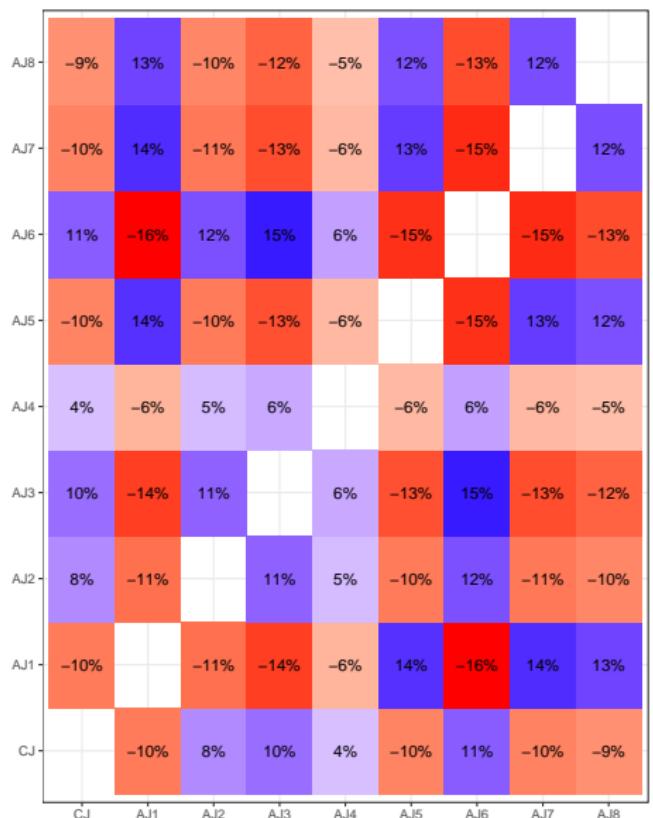
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# First Principal Component of Court Behavior

The most significant source of divided rulings is the familiar left/right split



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AP NEWS

9/11 A World Changed AP Top 25 College Football Poll Coronavirus pandemic Politics Sports Entertainment Photography

## Justice Ginsburg warns of more 5-4 decisions ahead

The New York Times

*Splitting 5 to 4, Supreme Court Backs Religious Challenge to Cuomo's Virus*

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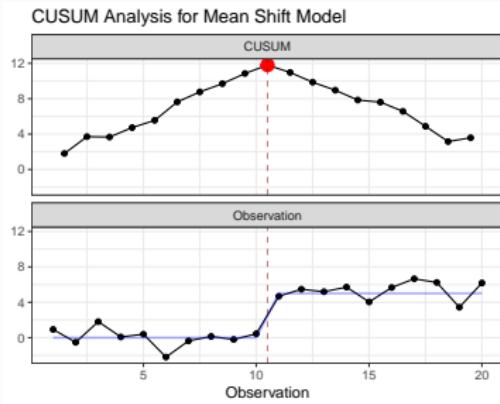
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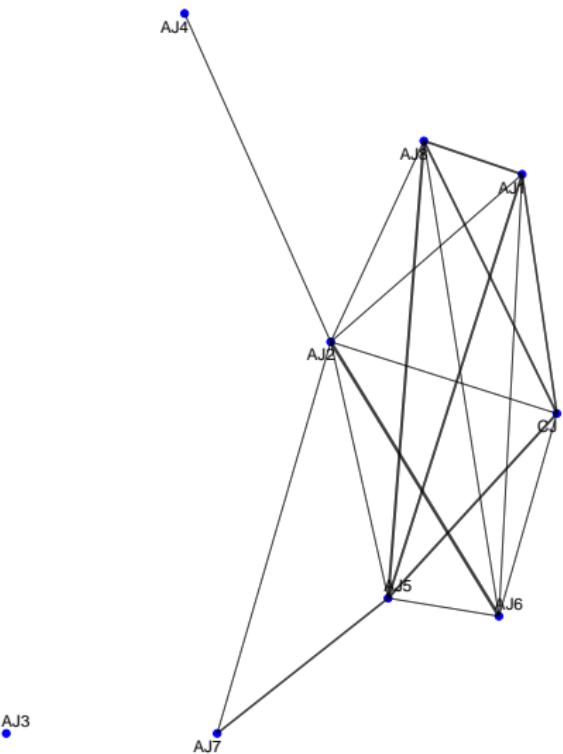
$$\text{cusum}(X)_t = \text{mean}(X_{<t}) - \text{mean}(X_{>t})$$



# First Principal Component of Tensor CUSUM Analysis

The most significant change in court dynamics is O'Connor / Alito (AJ2) seat

AJ8	9%	10%	-21%	-1%	3%	16%	-13%	4%	
AJ7	3%	3%	-7%	0%	1%	6%	-5%		4%
AJ6	-9%	-10%	23%	1%	-3%	-17%		-5%	-13%
AJ5	11%	12%	-27%	-1%	4%		-17%	6%	16%
AJ4	2%	3%	-6%	0%		4%	-3%	1%	3%
AJ3	-1%	-1%	1%		0%	-1%	1%	0%	-1%
AJ2	-15%	-17%		1%	-6%	-27%	23%	-7%	-21%
AJ1	7%		-17%	-1%	3%	12%	-10%	3%	10%
CJ		7%	-15%	-1%	2%	11%	-9%	3%	9%



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Also: Scalia / Gorsuch seat (AJ3) essentially unchanged

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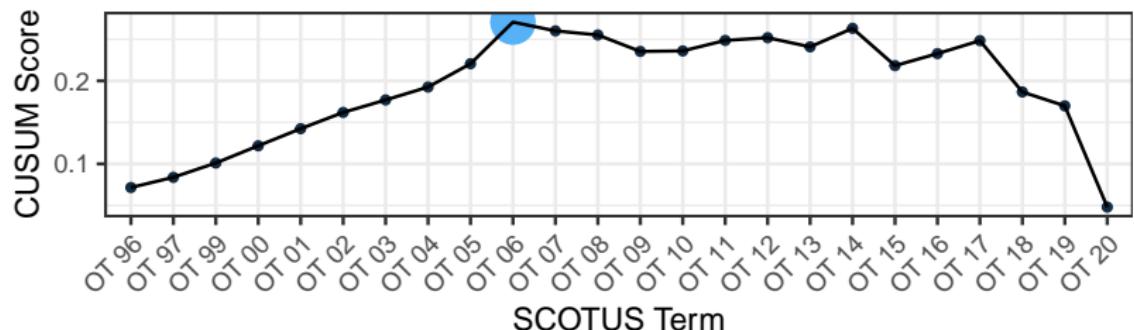
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# Semi-Symmetric PCA as a Flexible Pattern Recognition Tool

SS-PCA gives both **principal network** and **(time) loading vector**

For CUSUM analysis, loading vector identifies **when** change occurs

CUSUM Analysis of SCOTUS Consensus Dynamics  
CUSUM Analysis Identifies OT 05 as Major Turning Point



## Ongoing and Future Work

---

# Statistical Analysis of Partially Aligned Networks

Given two graphs  $\mathcal{G}_1, \mathcal{G}_2$  from (different) graphons, test difference

- Full Alignment: Yes! (Higher criticism, multiple binomial test; Ghoshdastidar *et al.*, AoS 2020)
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Approach:

- Adapt Smooth-and-Sort estimator (Chan & Airola, ICML 2014) for partial alignment
  - Message-passing step forces estimates for paired vertices to match
  - Statistical consistency
- Connections to partially paired  $t$ -test, permuted regression, etc.
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Related Work: “CONGA” (W., Michailidis, Roddenberry, ICASSP, 2021)

- Simultaneous community detection on two graphs via regularized PLS (sparsity + graph Laplacian smoothing) of graph signals

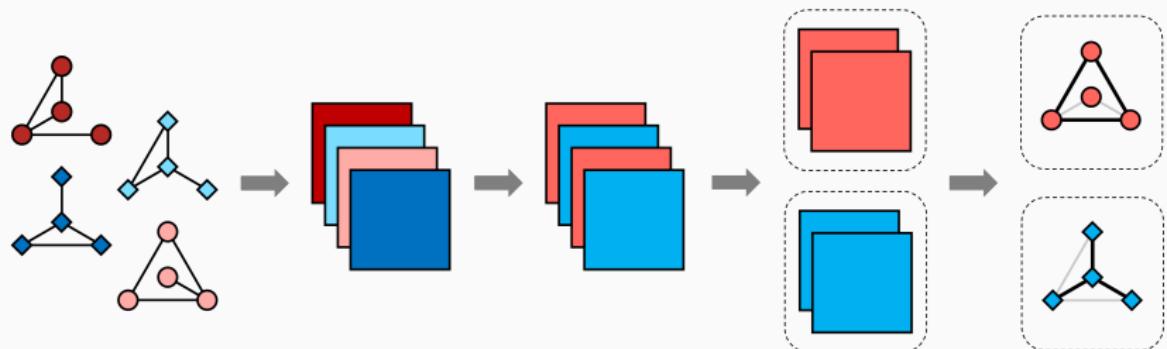
# Unsupervised Learning

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Methods for Regularized Matrix Decomposition and Clustering

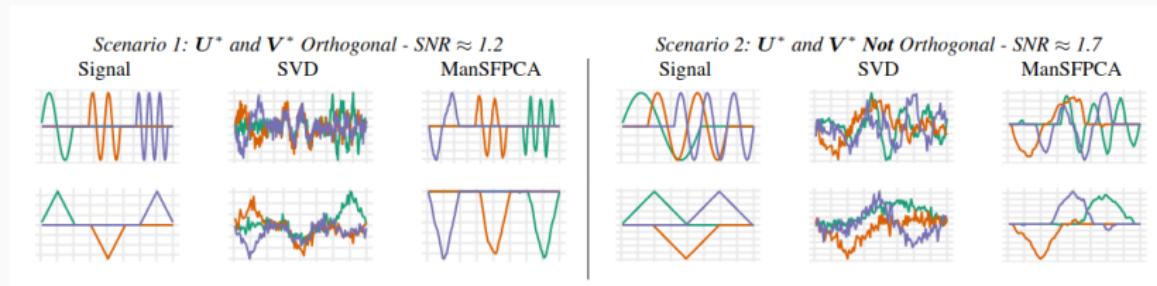
# Unsupervised Learning

## Methods for Regularized Matrix Decomposition and Clustering



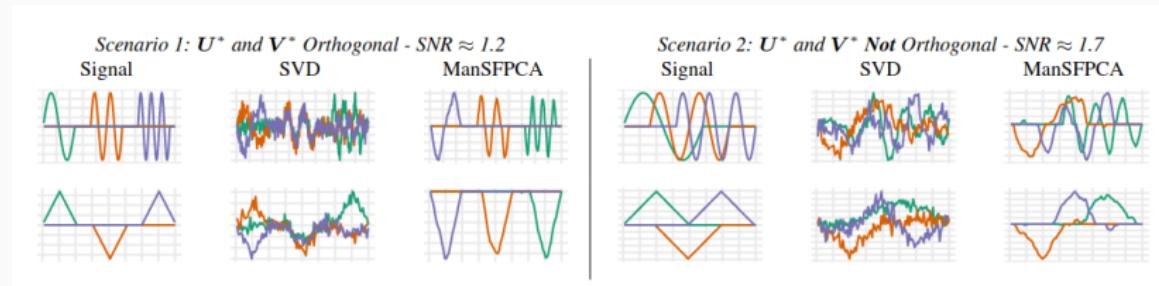
# Unsupervised Learning

# Methods for Regularized Matrix Decomposition and Clustering



# Unsupervised Learning

## Methods for Regularized Matrix Decomposition and Clustering



### Related Work:

- Sparse + Smooth PCA (Allen and W., *DSW*, 2019)
- Simultaneous regularized PCs via nonsmooth manifold optimization  
(W., *CAMSAP*, 2019)
- Convex clustering of networks (W. et al., 2022+)
- MoMA Software

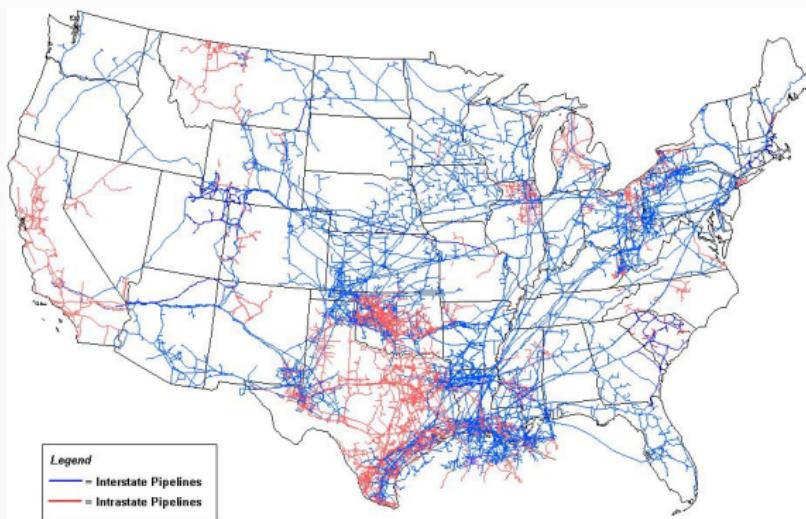
# Time Series Analysis

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Structured multivariate time series - finance, neuroscience, envirometrics

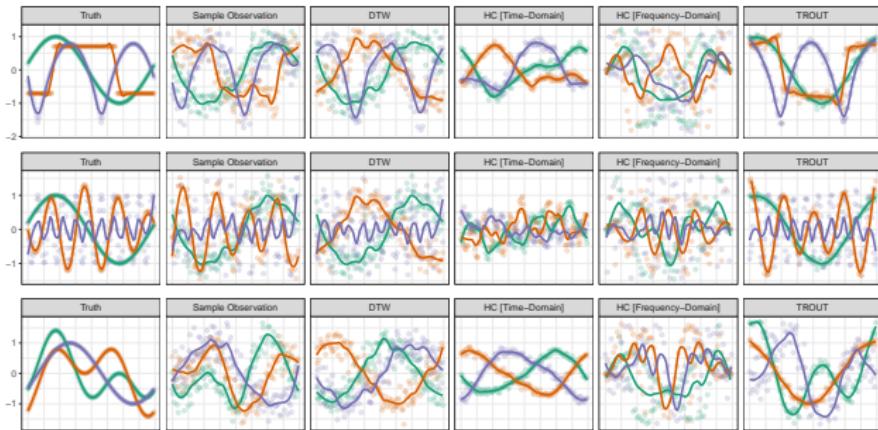
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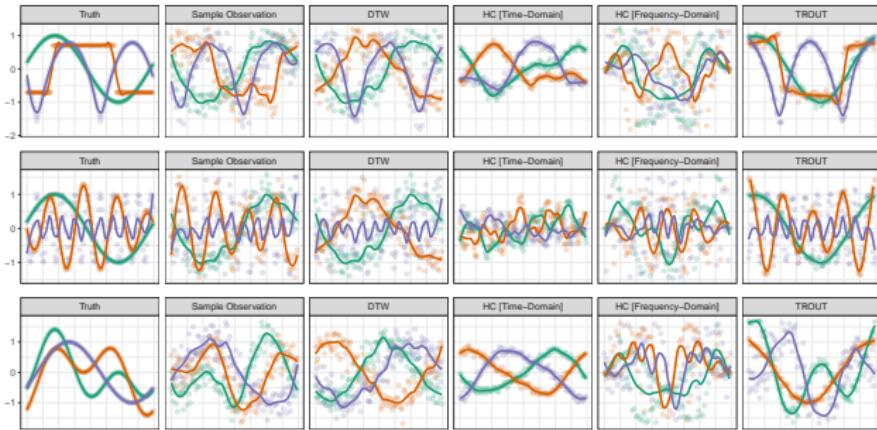
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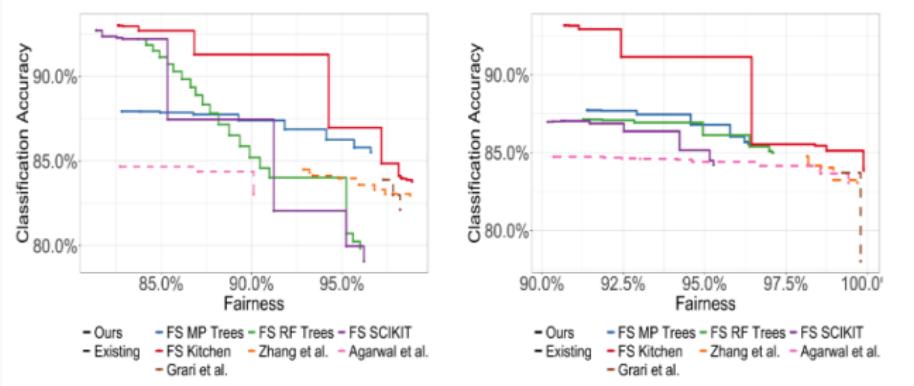


## Related Work:

- Econometric modeling of NG futures markets (W. et al., 2022+)
- Clustering of unaligned time series (W. & Michailidis, ICASSP 2021)
- Clustering + denoising time series (W. et al., DSLW, 2021)
- Complex-Valued Graphical Models of Time Series Spectra (W., 2022+)

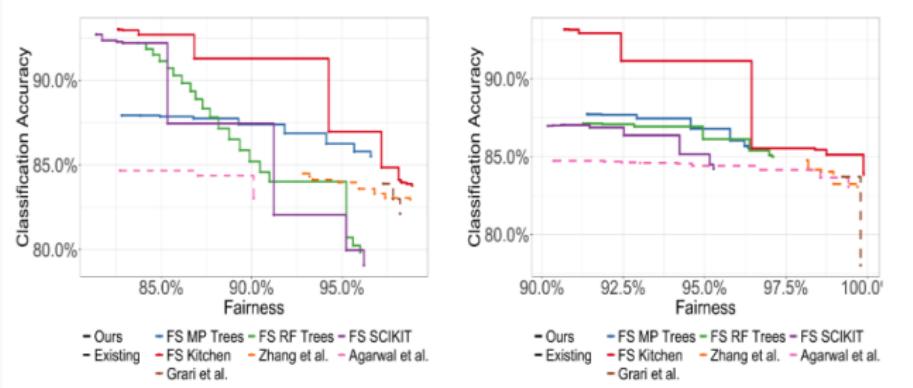
# Machine Learning Fairness

## Exploring Optimal Fairness-Accuracy Tradeoff (Pareto Frontier)



# Machine Learning Fairness

## Exploring Optimal Fairness-Accuracy Tradeoff (Pareto Frontier)



## Related Work:

- Measuring, Optimizing, and Testing Fairness-Accuracy Tradeoff (W. et al., 2022+)
- Fair PCA (W. and Allen, 2022+)
- Auditing individual fairness via metric learning (W. and Michailidis, 2022+)

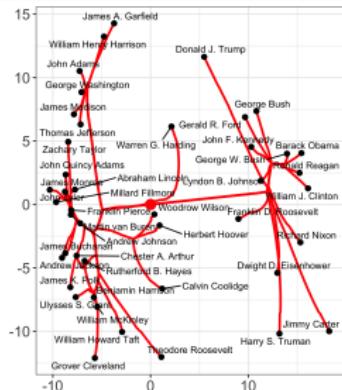
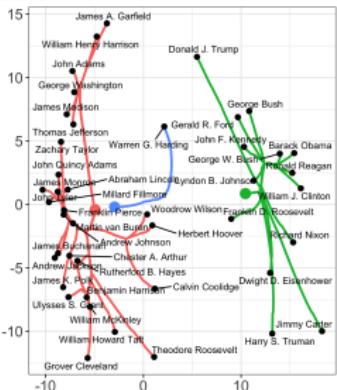
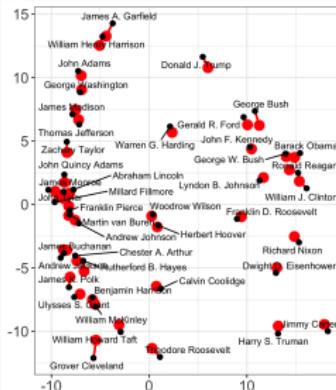
# Statistical Computing

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Development of efficient, robust, and “statistically sound” software

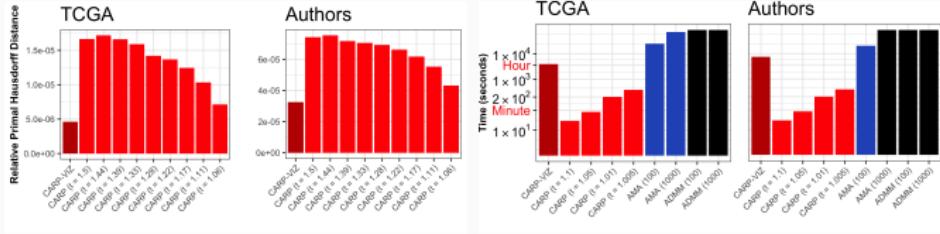
# Statistical Computing

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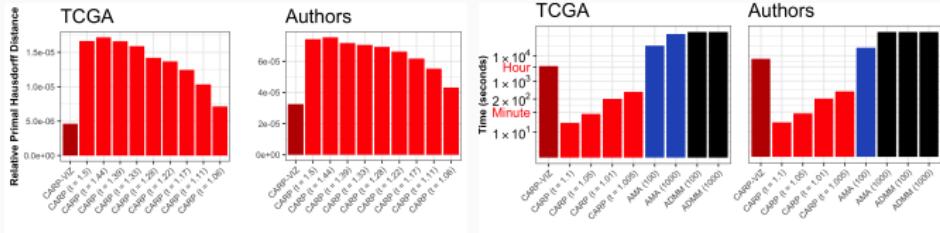
# Statistical Computing

Development of efficient, robust, and “statistically sound” software



# Statistical Computing

Development of efficient, robust, and “statistically sound” software



## Related Work:

- Efficient algorithms for computing regularization paths (W. et al., JCGS, 2020)
- Algorithms for higher-order convex clustering (W., DSW, 2019)
- Manifold optimization in unsupervised learning (W., CAMSAP, 2019)
- clustRviz, MoMA, ExclusiveLasso, etc. R packages

## Conclusions

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# Statistical Analysis of Multiple Networks



Network Tensor PCA – Network Science meets PCA:

# Statistical Analysis of Multiple Networks



Network Tensor PCA – Network Science meets PCA:

- Pattern recognition across **aligned** multiple networks

# Statistical Analysis of Multiple Networks



Network Tensor PCA – Network Science meets PCA:

- Pattern recognition across **aligned** multiple networks
- Trends, Variability, Changepoint Detection

# Statistical Analysis of Multiple Networks



Network Tensor PCA – Network Science meets PCA:

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- Efficient power method-inspired algorithm
  - Admits extensions for large, sparse, or streaming data

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  - Provable estimation consistency for non-convex problem
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## Backup Slides

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## Noise Model

Key notion of noise: operator noise of  $\mathcal{E}$  considered as mapping from  
 $\overline{\mathbb{B}}^T \times \mathcal{V}^{p \times r} \rightarrow \mathbb{R}_{\geq 0}$

$$\|\mathcal{E}\|_{r\text{-op}} = \max_{\mathbf{u}, \mathbf{V}} |\langle (\text{Tr}(\mathbf{V}^T \mathcal{E}_{..i} \mathbf{V}))_i, \mathbf{u} \rangle|$$

Deterministic upper bound:

$$\|\mathcal{E}\|_{r\text{-op}} \leq r\sqrt{T} \max_i \lambda_{\max}(\mathcal{E}_{..i})$$

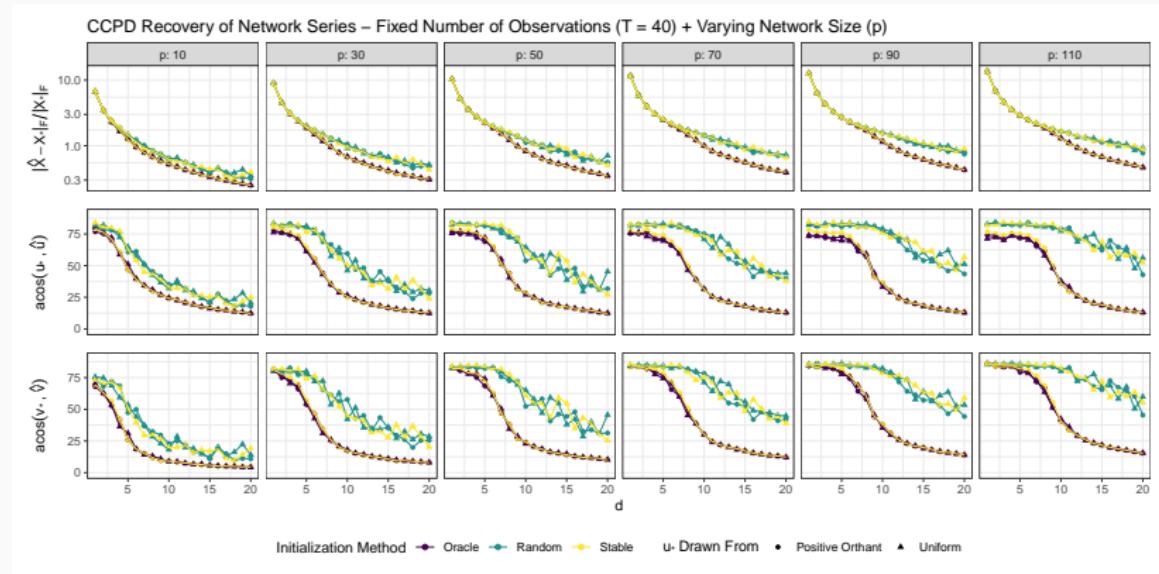
SS-Tensor Concentration bound:

$$\|\mathcal{E}\|_{r\text{-op}} \leq cr\sqrt{T}\sigma(\sqrt{p} + \sqrt{\log T} + \delta)$$

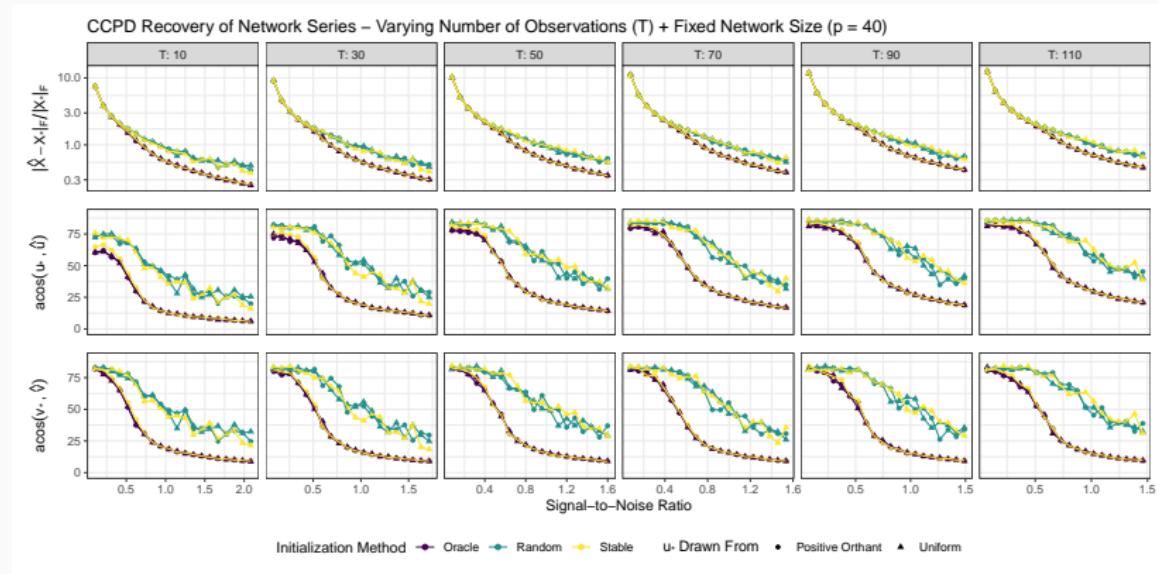
with probability at least  $1 - 4e^{-\delta^2}$

$c$  is small  $\Leftrightarrow c = 1$  for true Gaussians

# Simulations



# Simulations



## Stock Market Application

