Beyond matrices: nonparametric tensor completion via sign series

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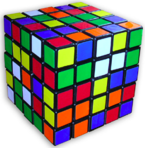
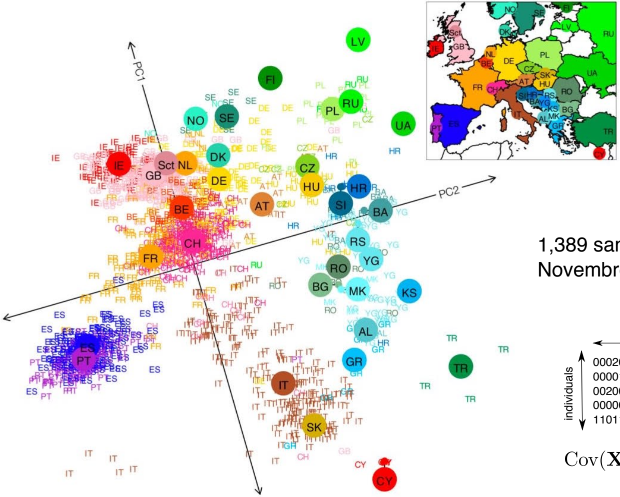
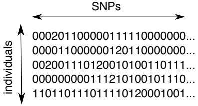
Joint work with Chanwoo Lee (3rd-year PhD student)



A successful story: PCA of Europeans



1,389 samples, ~ 200k SNPs
Novembre et al. (2008)



0002011000000111110000000...
0000110000000120110000000...
002001110120010100110111...
000000000111210100101110...
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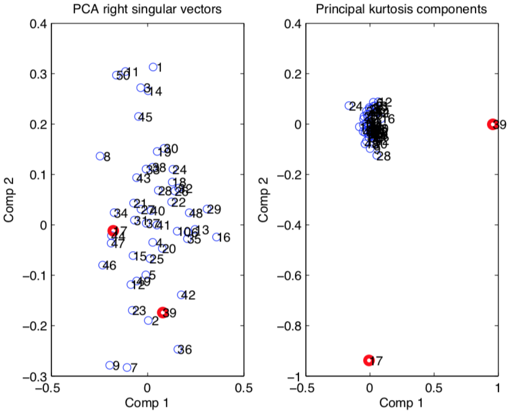
$$\mathrm{Cov}(\mathbf{X}) = \sum_{i=1}^{r} \lambda_i \mathbf{u}_i \mathbf{u}_i^T$$

Matrix methods are powerful, however...



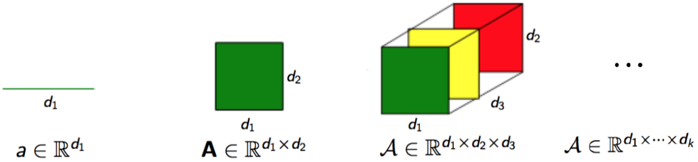
All Gaussian except points 17 and 39.

left: matrix PCA; right: principal components of kurtosis.

Figure credit: Jason Morton and Lek-Heng Lim (2009/2015).

What is a tensor?

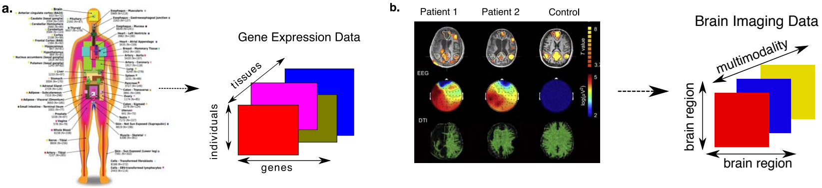
- Tensors are generalizations of vectors and matrices:



- An order-k tensor $\mathcal{A} = [\![a_{i_1 \ldots i_k}]\!] \in \mathbb{R}^{d_1 \times \cdots \times d_k}$ is a hypermatrix with dimensions $(d_1, \ldots, d_k)$ and entries $a_{i_1 \ldots i_k} \in \mathbb{R}$.
- This talk will focus on tensor of order 3 or greater, also known as higher-order tensors.

Tensors in genomics

- Many datasets come naturally in a multiway form.
- Multi-tissue, multi-individual gene expression measures could be organized as an order-3 tensor $\mathcal{A} = [\![a_{git}]\!] \in \mathbb{R}^{n_G \times n_I \times n_T}$.



Tensors in statistical modeling

"Tensors are the new matrices" that tie together a wide range of areas:

- Longitudinal social network data $\{\boldsymbol{Y}_t : t = 1, ..., n\}$
- Spatio-temporal transcriptome data
- Joint probability table of a set of variables $\mathbb{P}(X_1, X_2, X_3)$
- Higher-order moments in topic models
- Markov models for the phylogenetic tree $K_{1,3}$

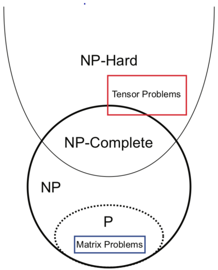
M. Yuan et al 2017, P. Hoff 2015, Montanari & Richard 2014

Anandkumar et al 2014, Mossel et al 2004, P. McCullagh 1987

Talk outline

Prohibitive Computational Complexity

Most higher-order tensor problems are NP-hard [Hillar & Lim, 2013].



Fortunately, the tensors sought in statistical and machine learning applications are often specially structured:

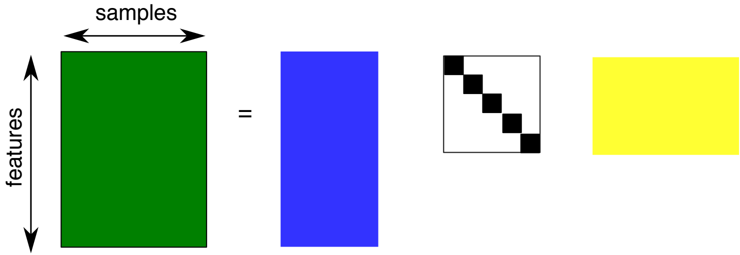
- Low-rankness
- Sparsity
- Non-negativity
- ...

This talk is based on

Beyond the Signs: Nonparametric Tensor Completion via Sign Series. Lee and W.

- arXiv:

Review: Matrix SVD for biclustering



$$\mathbf{X} = \mathbf{U} \quad \Lambda \quad \mathbf{V}^T$$

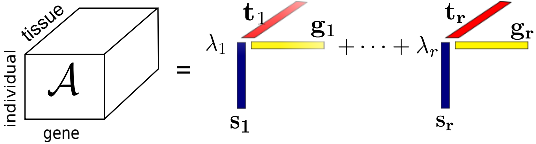
$$= \sum_{i=1}^{r} \lambda_i \mathbf{u}_i \mathbf{v}_i^T$$

- Columns of $\mathbf{U}$ describe patterns across samples
- Columns of $\mathbf{V}^T$ describe patterns across genes

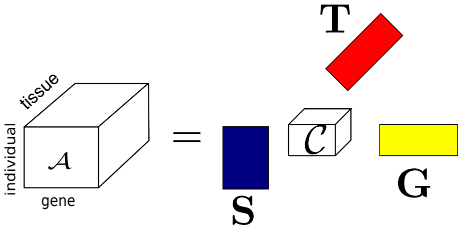
Y Kluger et al, Genome Research (2003). 13(4): 703-71
Data Science Specialization (COURSERA) by Brian Caffo and Jeff Leek

Various notions of low-rankness

- Canonical polyadic (CP) low-rankness: $\mathcal{A} = \sum_{r=1}^{R} \lambda_r \boldsymbol{s}_r \otimes \boldsymbol{g}_r \otimes \boldsymbol{t}_r$.

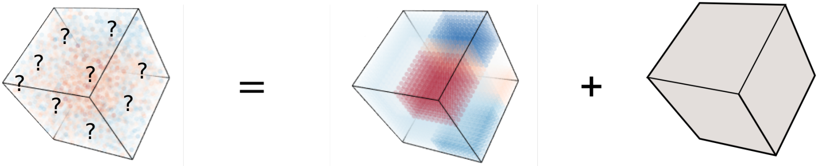


- Tucker low-rankness: $\mathcal{A} = \mathcal{C} \times_1 \boldsymbol{S} \times_2 \boldsymbol{G} \times_3 \boldsymbol{T}$.



- Others: tensor train [Oseledet '11], tensor block model [W. & Zeng '19; Han, Luo, W. et al '20], etc.

Setup: signal plus noise model



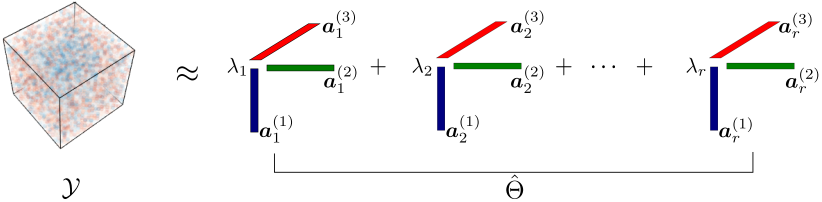
$\underbrace{\mathcal{Y}}_{\text{Data tensor}}$ $\underbrace{\Theta}_{\text{Signal tensor}}$ $\underbrace{\mathcal{E}}_{\text{Noise tensor}}$

We focus on the two problems:

- Nonparametric tensor estimation: How to estimate the signal tensor Θ under a wide range of structures?
- Tensor completion: How many observed tensor entries do we need in order for consistent recovery?

Inadequacies of low-rank models

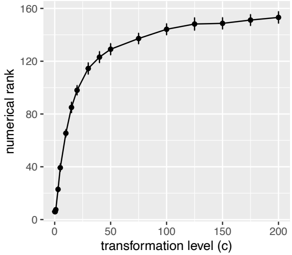
- Classical low-rank models (Jain & Oh' 14; Motanari & Sun '18):



- Two limitations of classical low-rank models:
  1. Sensitivity to order-preserving transformation.
  2. Inadequacy for special structures.

Inadequacies of low-rank models

- Tensor rank is sensible to order-preserving transformation.



$$\Theta = \frac{1}{1+\exp(-c\,(\mathcal{Z}))}, \quad \text{where}$$

$$\mathcal{Z} = \boldsymbol{a}^{\otimes 3} + \boldsymbol{b}^{\otimes 3} + \boldsymbol{c}^{\otimes 3}$$

$\Rightarrow$ Θ is high-rank but $\mathcal{Z}$ is low-rank.

Inadequacies of low-rank models

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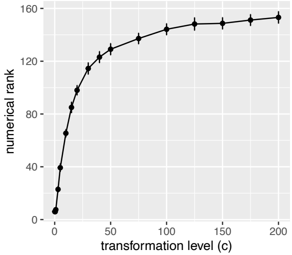

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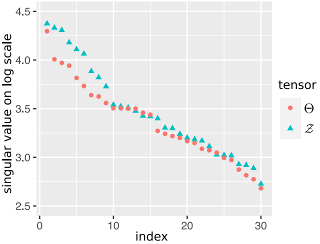
- Low-rank model fails to address several important structures.



$$\Theta = \log(1+\mathcal{Z}), \quad \text{where}$$

$$\mathcal{Z} = [\![\mathcal{Z}(i,j,k)]\!] = \frac{1}{d}\max(i,j,k).$$

$\Rightarrow$ Both Θ and $\mathcal{Z}$ are full rank.

The matrix analogy of Θ was studied in the context of graphon analysis by Chan and Airoldi (2014).

Related work and our contributions

- **Low-rank tensor estimation** (Anandkumar et al. 2014; Montanari and Sun 2018; Cai et al. 2019) focuses on the regime of fixed rank r growing dimension d. ⇒ low-rank assumption is often violated in practice.
- **High-rank matrix estimation** was studied under nonlinear models (Ganti et al., 2015) and subspace clustering (Ongie et al., 2017; Fan and Udell, 2019). ⇒ tensors are more challenging as rank may exceed dimension.

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Our contributions

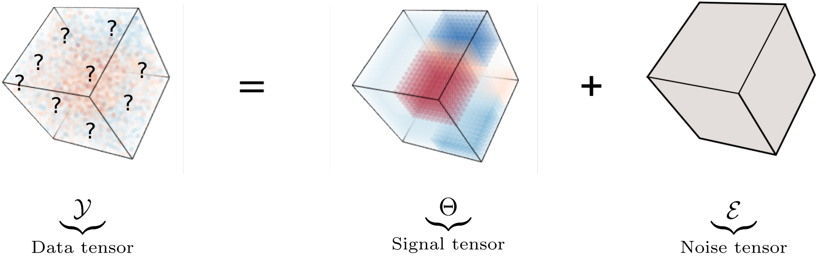
- We develop a new model called sign representable tensors to fill the gap between parametric (low-rank) and nonparametric (high-rank) tensors.
- Our tensor estimate is provably reductable to a series of classifications. ⇒ a divide-and-conquer nature for efficient computation.

Why sign matters?

For any bounded tensor $\Theta \in [-1,1]^{d_1\times\cdots\times d_K}$,

$$\Theta \approx \sum_{\pi\in\mathcal{H}} \operatorname{sgn}(\Theta-\pi), \quad \text{where} \quad \mathcal{H}=\left\{-1,\ldots,-\frac{1}{H},0,\frac{1}{H},\ldots,1\right\}.$$

- We do not observe Θ; instead, we observe a noisy incomplete version $\mathcal{Y}$.
- How to estimate the signal tensor Θ given data tensor $\mathcal{Y}$?

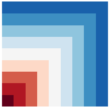


Sign rank

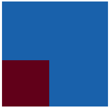
- Key ideas: we use a local (nonparametric) notion of "low-rankness" that allows a broader family of signal tensors.
- Two tensors are sign equivalent, denoted $\Theta \simeq \Theta'$, if $\text{sgn}(\Theta) = \text{sgn}(\Theta')$.
- Define the sign rank by

$$\text{srank}(\Theta) = \min\{\text{rank}(\Theta') \colon \Theta' \simeq \Theta,\ \Theta' \in \mathbb{R}^{d_1 \times \cdots \times d_K}\}.$$

$\Theta =$



$,\quad \text{sgn}(\Theta) =$



$$\Longrightarrow \begin{array}{c} \text{rank}(\Theta) = d \\ \text{srank}(\Theta) = 2 \end{array}$$

- For any strictly monotonic function $g \colon \mathbb{R} \to \mathbb{R}$ with $g(0) = 0$,

$$\text{srank}(\Theta) \le \text{rank}(g(\Theta)).$$

Sign representable tensors

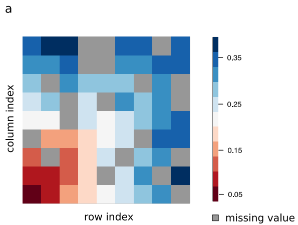
Sign representable tensors

A tensor Θ is called r-sign representable if the tensor $(\Theta - \pi)$ has sign rank bounded by r for all $\pi \in [-1, 1]$.

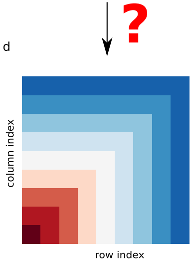
- Most existing structured tensors belong to sign representable family:
  - Low-rank CP tensors, Tucker tensors, stochastic tensor block models.
  - High-rank tensors from GLM, single index models.
  - Earlier example $\Theta(i_1, \ldots, i_K) = \log(1 + \max(i_1, \ldots, i_K))$ is 2-sign representable ⇒ conclusion extends to general max/min hypergraphon models.
- We propose the signal tensor family

$$\Theta \in \mathscr{P}_{\text{sgn}}(r) := \{\Theta \colon \text{srank}(\Theta - \pi) \leq r \text{ for all } \pi \in [-1, 1]\}.$$

Our solution: sign signal helps!



noisy and incomplete observation



recovered high-rank signals

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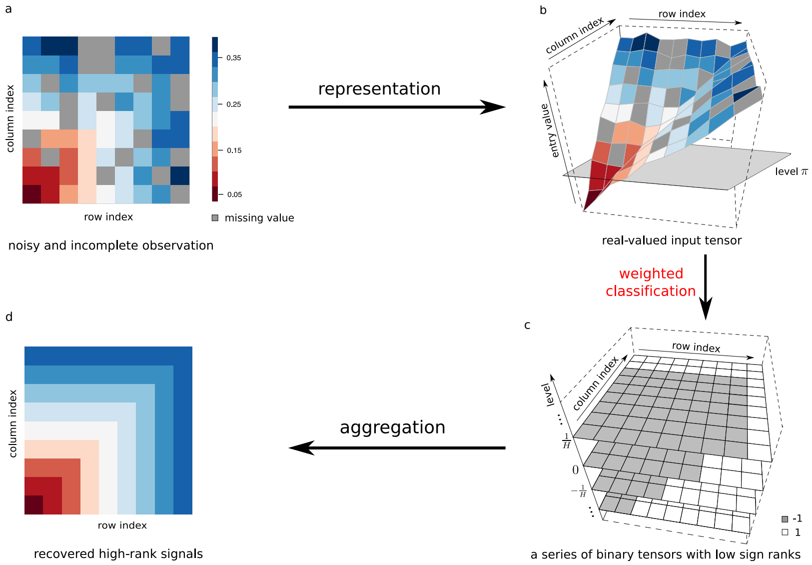


noisy and incomplete observation

representation

real-valued input tensor

weighted classification

a series of binary tensors with low sign ranks

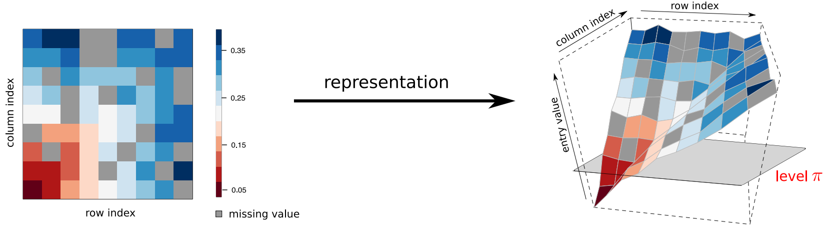
aggregation

recovered high-rank signals

Sign representation

- We observe a noisy incomplete tensor $\mathcal{Y}_\Omega \in [-1,1]^{d_1\times\cdots\times d_K}$ with observed index set $\Omega \in [d_1]\times\cdots\times[d_K]$ under uniform sampling scheme.
- We dichotomize the data into a series of sign tensors:

$$\{\textsf{sgn}(\mathcal{Y}_\Omega-\pi)\}_{\pi\in\mathcal{H}}, \quad \text{where } \mathcal{H}=\left\{-1,\ldots,-\frac{1}{H},0,\frac{1}{H},\ldots,1\right\}.$$



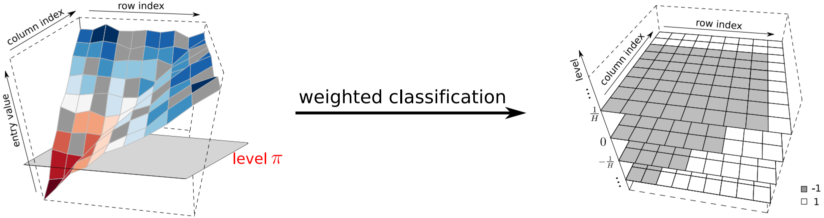
noisy and incomplete observation

real-valued input tensor

Sign estimation via weighted classification

- We estimate $\mathrm{sgn}(\Theta - \pi)$ through $\mathrm{sgn}(\mathcal{Y}_\Omega - \pi)$ via weighted classification.
- Objective function of weighted classification is

$$L(\mathcal{Z}, \mathcal{Y}_\Omega - \pi) = \frac{1}{|\Omega|} \sum_{\pi \in \Omega} \underbrace{|\mathcal{Y}(\omega) - \pi|}_{\text{weight}} \times \underbrace{|\mathrm{sgn}(\mathcal{Z}(\omega)) - \mathrm{sgn}(\mathcal{Y}(\omega) - \pi)|}_{\text{classification loss}}$$



real-valued input tensor

a series of binary tensors with low sign ranks

Identification for sign tensor estimation

α-smoothness of signal tensor

For fixed π, Θ is α-smooth if there exist $\alpha = \alpha(\pi) > 0, c = c(\pi) > 0$, s.t.

$$\sup_{0 \leq t < \rho(\pi,\mathcal{N})} \frac{\mathbb{P}_{\omega \sim \Pi}[|\Theta(\omega) - \pi| \leq t]}{t^{\alpha}} \leq c,$$

where $\rho(\pi,\mathcal{N}) = \min_{\pi' \in \mathcal{N}} |\pi - \pi'|$ and $\mathcal{N} = \{\pi \colon \mathbb{P}(\Theta(\omega) = \pi) \neq 0\}$. If α and c are global constants for all* π's, we call Θ is α-globally smooth.

* except for a finite number of π's.

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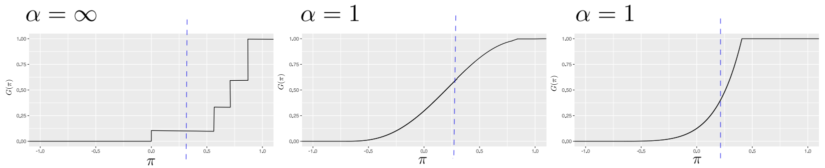
Intuition: sign recovery is harder at levels where point mass concentrates.

Rate depends on the behavior of CDF function $G(\pi) = \mathbb{P}_{\omega \sim \Pi}[\Theta(\omega) \leq \pi]$.



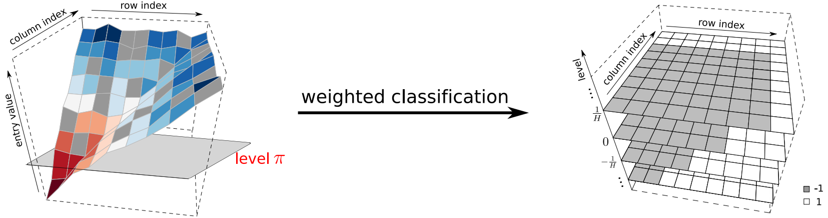
Identification for sign tensor estimation

- If Θ is α-smooth $(\alpha > 0)$, we have an unique optimizer such that

$$\textsf{sgn}(\Theta - \pi) = \mathop{\arg\min}_{\mathcal{Z}:\ \textsf{rank}(\mathcal{Z}) \leq r} \mathbb{E}_{\mathcal{Y}_\Omega} L(\mathcal{Z}, \mathcal{Y}_\Omega - \pi).$$

- We obtain a series of optimizers $\{\hat{\mathcal{Z}}_\pi\}_{\pi \in \mathcal{H}}$ as

$$\hat{\mathcal{Z}}_\pi = \mathop{\arg\min}_{\mathcal{Z}:\ \textsf{rank}(\mathcal{Z}) \leq r} L(\mathcal{Z}, \mathcal{Y}_\Omega - \pi).$$



real-valued input tensor

a series of binary tensors with low sign ranks

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*Uniqueness up to sign equivalence, meaning the optimizer $\Theta_{\text{opt}} \simeq \textsf{sgn}(\Theta - \pi)$.

Sign tensor estimation error

- For two tensor Θ_1, Θ_2, define $\text{MAE}(\Theta_1, \Theta_2) = \mathbb{E}_{\omega \in \Pi}|\Theta_1(\omega) - \Theta_2(\omega)|$.

Sign tensor estimation for fixed π (Lee and W. 2021)

Suppose $\Theta \in \mathscr{P}_{\text{sgn}}(r)$ and $\Theta(\omega)$ is α-smooth for fixed π. Let $d_{\max} = \max_{k \in [K]} d_k$. Then, with very high probability over $\mathcal{Y}_\Omega$,

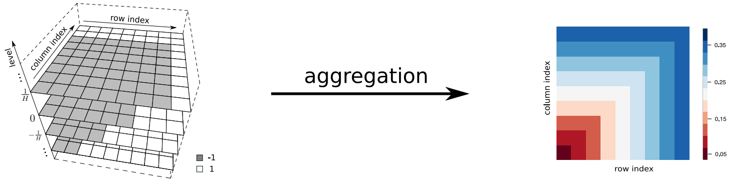
$$\text{MAE}(\text{sgn}\hat{\mathcal{Z}}_\pi, \text{sgn}(\Theta - \pi)) \lesssim \left(\frac{d_{\max} r}{|\Omega|}\right)^{\frac{\alpha}{\alpha+2}}.$$

- Sign estimation error shows a polynomial decay with $|\Omega|$.
- Best rate attains at $\alpha = \infty$ for stochastic tensor block models.

From sign to signal estimation

- Aggregation of sign tensors from weighted classification yields the possibly high-rank signal tensor estimate:

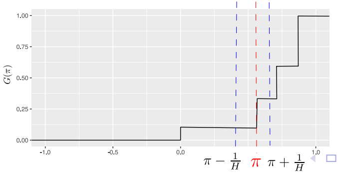
$$\hat{\Theta} = \frac{1}{2H+1} \sum_{\pi \in \mathcal{H}} \text{sgn} \hat{\mathcal{Z}}_{\pi}.$$



a series of binary tensors with low sign ranks

recovered high-rank signals

- Signal tensor estimation is robust to a few off-target classifications.



Signal tensor estimation error

Tensor estimation error (Lee and W. 2021)

Suppose $\Theta \in \mathscr{P}_{\text{sgn}}(r)$ and $\Theta(\omega)$ is α-globally smooth. Then, with very high probability over $\mathcal{Y}_\Omega$,

$$\text{MAE}(\hat{\Theta}, \Theta) \lesssim \underbrace{\left(\frac{d_{\max} r}{|\Omega|}\right)^{\frac{\alpha}{\alpha+2}}}_{\text{error inherited from sign estimation}} + \underbrace{\frac{1}{H}}_{\text{Bias}} + \underbrace{\frac{H d_{\max} r}{|\Omega|}}_{\text{Variance}}.$$

In particular, setting $H \asymp \left(\frac{|\Omega|}{d_{\max} r}\right)^{1/2}$ yields the error bound

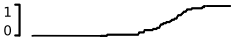
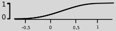
$$\text{MAE}(\hat{\Theta}, \Theta) \lesssim \left(\frac{d_{\max} r}{|\Omega|}\right)^{\frac{\alpha}{\alpha+2} \vee \frac{1}{2}}.$$

- Sample requirement for tensor completion:

$$\text{MAE}(\hat{\Theta}, \Theta) \to 0, \text{ as } \frac{|\Omega|}{d_{\max} r} \to \infty.$$

Comparison of estimation error versus dimension

- We simulate signal tensors under a wide range of complexity.

Simulation	Signal Tensor Θ	Rank	Sign Rank	Global α	CDF	Noise
1	$\mathcal{C} \times \boldsymbol{M}_1 \times \boldsymbol{M}_2 \times \boldsymbol{M}_3$	3^3	$\leq 3^3$	∞		Uniform $[-0.3, 0.3]$
2	$\lvert \boldsymbol{a} \otimes \mathbf{1} \otimes \mathbf{1} - \mathbf{1} \otimes \boldsymbol{a} \otimes \mathbf{1} \rvert$	d	≤ 3	1		Normal $\mathcal{N}(0, 0.15)$
3	$\log(0.5 + Z_{\max})$	$\geq d$	2	1		Uniform $[-0.1, 0.1]$
4	$2.5 - \exp(\mathcal{Z}_{\min}^{1/3})$	$\geq d$	2	1		Normal $\mathcal{N}(0, 0.15)$

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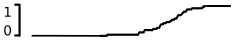
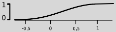
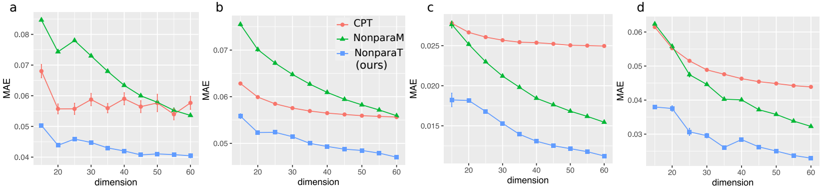
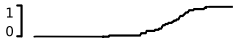
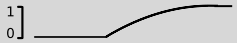
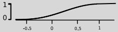
1	$\mathcal{C}\times\boldsymbol{M}_1\times\boldsymbol{M}_2\times\boldsymbol{M}_3$	3^3	$\leq 3^3$	∞		Uniform $[-0.3, 0.3]$
2	$\lvert\boldsymbol{a}\otimes\mathbf{1}\otimes\mathbf{1}-\mathbf{1}\otimes\boldsymbol{a}\otimes\mathbf{1}\rvert$	d	≤ 3	1		Normal $\mathcal{N}(0, 0.15)$
3	$\log(0.5+Z_{\max})$	$\geq d$	2	1		Uniform $[-0.1, 0.1]$
4	$2.5-\exp(\mathcal{Z}_{\min}^{1/3})$	$\geq d$	2	1		Normal $\mathcal{N}(0, 0.15)$

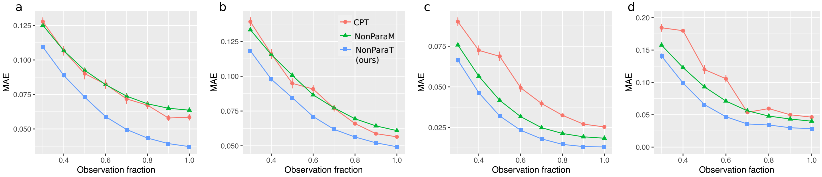
- Our method (NonparaT) achieves the best performance, whereas the second best method is low-rank CP tensor (CPT) for models 1-2, and matrix version of our method (NonParaM) for models 3-4.



Estimation error versus observation fraction

Simulation	Signal Tensor Θ	Rank	Sign Rank	Global α	CDF	Noise
1	$\mathcal{C}\times\boldsymbol{M}_1\times\boldsymbol{M}_2\times\boldsymbol{M}_3$	3^3	$\leq 3^3$	∞		Uniform $[-0.3, 0.3]$
2	$\lvert\boldsymbol{a}\otimes\mathbf{1}\otimes\mathbf{1}-\mathbf{1}\otimes\boldsymbol{a}\otimes\mathbf{1}\rvert$	d	≤ 3	1		Normal $\mathcal{N}(0, 0.15)$
3	$\log(0.5+Z_{\max})$	$\geq d$	2	1		Uniform $[-0.1, 0.1]$
4	$2.5-\exp(\mathcal{Z}_{\min}^{1/3})$	$\geq d$	2	1		Normal $\mathcal{N}(0, 0.15)$

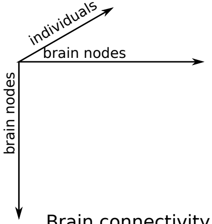
- Our method (NonparaT) achieves the best performance in completion.



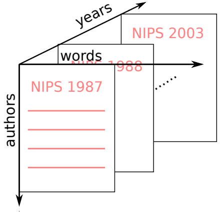
Data application

We apply our method to three datasets:

- The human brain connectivity data (Wang et al., 2017) consists of 68 brain regions for 114 individuals along with their IQ scores.
- The NIPS dataset (Globerson et al., 2007) consists of word occurrence counts in papers published from 1987 to 2003.
- The 3-channel image data is from licensed google image file.



Brain connectivity



NIPS data

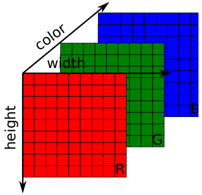
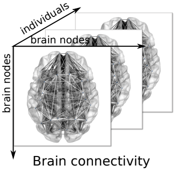


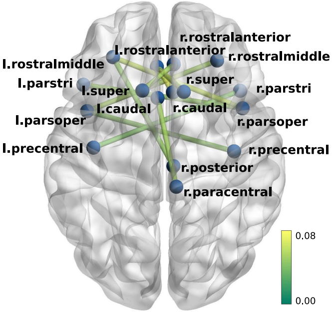
Image data

Data application: Brain connectivity

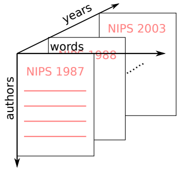


- The MRN-114 human brain connectivity data consists of 68 brain regions for 114 individuals along with their IQ scores .
- Data tensor $\mathcal{Y} \in \{0,1\}^{68\times 68\times 114}$.

- We examine the estimated signal tensor $\hat{\Theta}$.
- Top 10 brain edges based on regression analysis show inter-hemisphere connections.



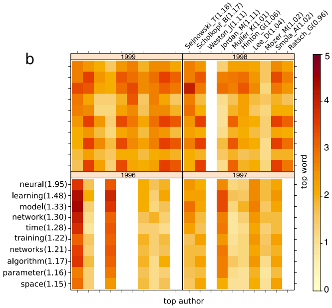
Data application: NIPS



NIPS data

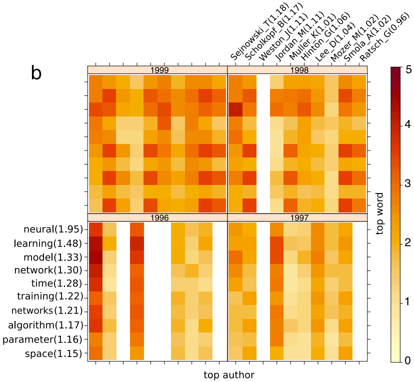
- The NIPS dataset consists of word occurrence counts in papers published from 1987 to 2003.
- Data tensor $\mathcal{Y} \in \mathbb{R}^{100 \times 200 \times 17}$.

- We examine the estimated signal tensor $\hat{\Theta}$.
- Most frequent words are consistent with the active topics.
- Strong heterogeneity among word occurrences across authors and years.



Data application: NIPS

- Top words: *neural* (1.95), *learning* (1.48), *network* (1.21), *training* (1.22), *parameter (1.16)*.
- Top authors: *T. Sejnowski* (1.18), *B. Schölkopf* (1.17), *M. Jordan* (1.11), and *G. Hinton* (1.06),
- Top combinations:
  (*training*, *algorithm*) × (*B. Schölkopf*, *A. Smola*) × (1998, 1999),
  (*model*) × (*M. Jordan*) × (1996).
- Similar word patterns in 1998-1999:
  (*B. Schölkopf*, *Möller K*, *A. Smola*, *G. Rätsch*, *J. Weston*) ⇒ Co-authors.



Numbers in parentheses denote marginal averages based on $\hat{\Theta}$

details

Data application: Brain connectivity + NIPS

- Our method achieves lower test error than low-rank tensor methods.

MRN-114 brain connectivity dataset					
Method	$r = 3$	$r = 6$	$r = 9$	$r = 12$	$r = 15$
NonparaT (Ours)	**0.18**(0.001)	**0.14**(0.001)	**0.12**(0.001)	**0.12**(0.001)	**0.11**(0.001)
Low-rank CPT	0.26(0.006)	0.23(0.006)	0.22(0.004)	0.21(0.006)	0.20(0.008)
NIPS word occurrence dataset					
Method	$r = 3$	$r = 6$	$r = 9$	$r = 12$	$r = 15$
NonparaT (Ours)	**0.18**(0.002)	**0.16**(0.002)	**0.15**(0.001)	**0.14**(0.001)	**0.13**(0.001)
Low-rank CPT	0.22(0.004)	0.20(0.007)	0.19(0.007)	0.17(0.007)	0.17(0.007)
Naive imputation (Baseline)	0.32(.001)				

Table: MAE comparison in the brain data and NIPS data based on 5-folded cross-validations. Standard errors are reported in parenthesis.

Data application: Image

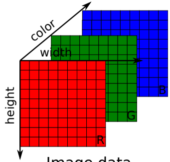
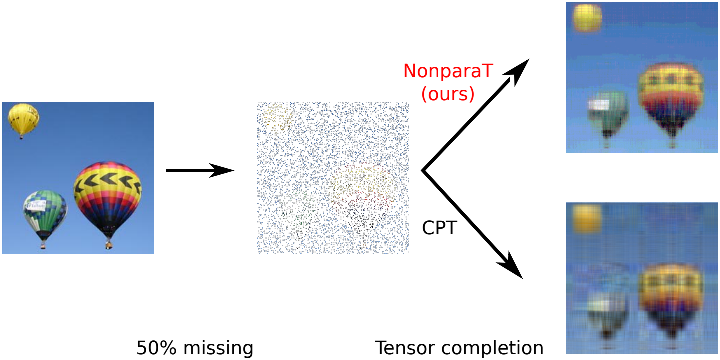


Image data

- The original data is from licensed google image file.
- data tensor $\mathcal{Y} \in [0,1]^{217\times 217\times 3}$.
- We assess completion performance by sampling 50% entries in the original image tensor.



NonparaT (ours)

CPT

50% missing

Tensor completion

Summary

Tensor analysis provides a rich source of

- fundamental problems in data science.
- new tools for long-standing questions.
- potentials for new applications.

Our general strategy is to carve out a broad range of specially-structured tensors that are useful in practice, and to develop efficient statistical methods for analyzing these high-dimensional tensor data.

References:

- Beyond the sign: nonparametric tensor completion from sign series.

Acknowledgment: NSF DMS 1915978 and Grant from Wisconsin Alumni Research Foundation.

Appendix

Algorithm 1 Nonparametric tensor completion

```
Input: Noisy and incomplete data tensor $\mathcal{Y}_\Omega$, rank $r$, resolution parameter $H$.
for $\pi \in \mathcal{H} = \{-1, \ldots, -\frac{1}{H}, 0, \frac{1}{H}, \ldots, 1\}$ do
    Random initialization of tensor factors $\boldsymbol{A}_k = [\boldsymbol{a}_1^{(k)}, \ldots, \boldsymbol{a}_r^{(k)}] \in \mathbb{R}^{d_k \times r}$ for all $k \in [K]$.
    while not convergence do
        for $k = 1, \ldots, K$ do
            Update $\boldsymbol{A}_k$ while holding others fixed:
            $\boldsymbol{A}_k \leftarrow \arg\min_{\boldsymbol{A}_k \in \mathbb{R}^{d_k \times r}} \sum_{\omega \in \Omega} |\mathcal{Y}(\omega) - \pi| F(\mathcal{Z}(\omega)\mathrm{sgn}(\mathcal{Y}(\omega) - \pi))$,
            where $F(\cdot)$ is the large-margin loss, and $\mathcal{Z} = \sum_{s \in [r]} \boldsymbol{a}_s^{(1)} \otimes \cdots \otimes \boldsymbol{a}_s^{(K)}$ is a rank-$r$ tensor.
        end for
    end while
    Return $\mathcal{Z}_\pi \leftarrow \sum_{s \in [r]} \boldsymbol{a}_s^{(1)} \otimes \cdots \otimes \boldsymbol{a}_s^{(K)}$.
end for
Output: Estimated signal tensor $\hat{\Theta} = \frac{1}{2H+1} \sum_{\pi \in \mathcal{H}} \mathrm{sgn}(\mathcal{Z}_\pi)$.
```

NIPS dataset

1998:

- Kernel PCA and De-Noising in Feature Spaces. Sebastian Mika, **B. Schölkopf**, **A. Smola**, **K. Müller**, M. Scholz, **G. Rätsch**
- Shrinking the Tube: A New Support Vector Regression Algorithm. **B. Schölkopf**, P. Bartlett, **A. Smola**, R. C. Williamson
- Semiparametric Support Vector and Linear Programming Machines. **A. Smola**, T-T. Frieb, **B. Schölkopf**
- Regularizing AdaBoost. **G. Rätsch**, T. Onoda, **K. Müller**

1999:

- v-Arc: Ensemble Learning in the Presence of Outliers. **G. Rätsch**, **B. Schölkopf**, **A. Smola**, **K. Müller**, T. Onoda, S. Mika
- Invariant Feature Extraction and Classification in Kernel Spaces. S. Mika, **G. Rätsch**, **J. Weston**, **B. Schölkopf**, **A. Smola**, **K Müller**
- Support Vector Method for Novelty Detection. **B. Schölkopf**, R. C. Williamson, **A. Smola**, J. S. Taylor, J. Platt.

1996:

- A Variational Principle for Model-based Morphing. L. Saul, **M. Jordan**
- Hidden Markov Decision Trees. **M. Jordan**, Z. Ghahramani, L. Saul
- Triangulation by Continuous Embedding. M. Meila, **M. Jordan**
- Recursive Algorithms for Approximating Probabilities in Graphical Models. T. Jaakkola, **M. Jordan**

Back to NIPS analysis

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