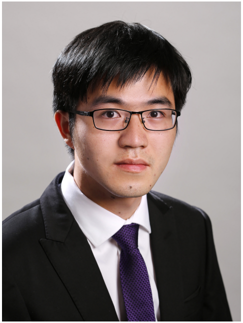
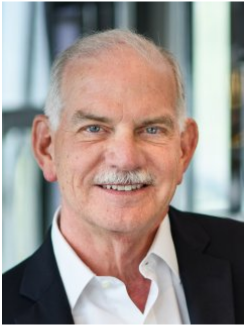
Uncertainty quantification for nonconvex tensor completion

Yuxin Chen

Electrical Engineering, Princeton University

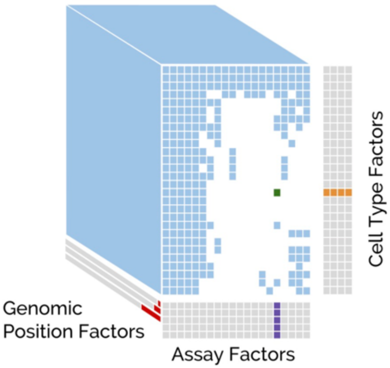


Changxiao Cai
Princeton EE

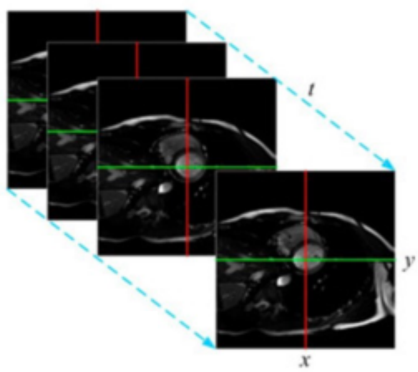


H. Vincent Poor
Princeton EE

Ubiquity of high-dimensional tensor data

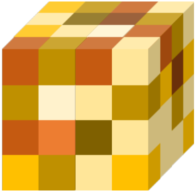


computational genomics
— *fig. credit: Schreiber et al. 19*



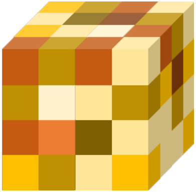
dynamic MRI
— *fig. credit: Liu et al. 17*

Challenges in tensor reconstruction



a tensor of interest

Challenges in tensor reconstruction



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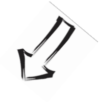
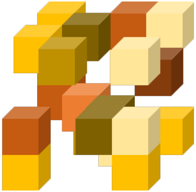
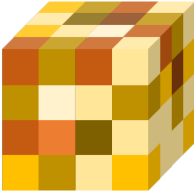




mising data

Challenges in tensor reconstruction



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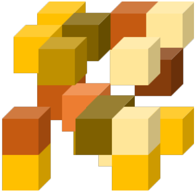
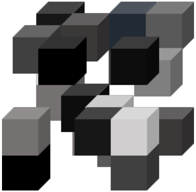
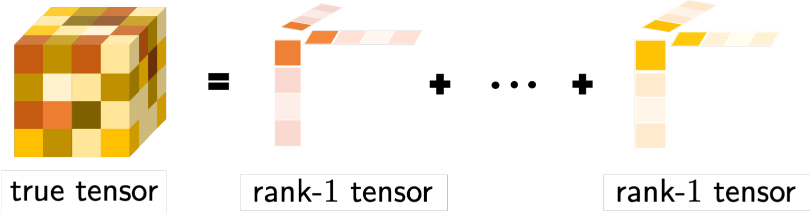


mising data



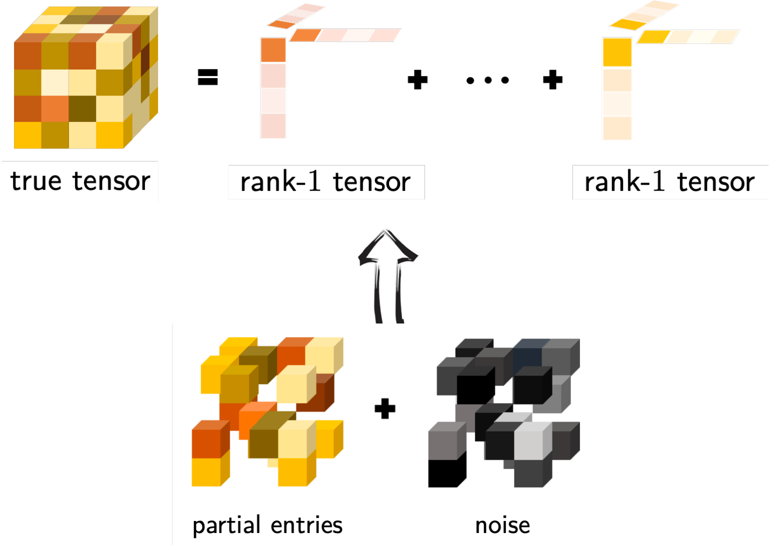
noise

Key to enabling reliable reconstruction from incomplete & noisy data:

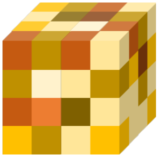


— **exploiting low (CP) rank structure**

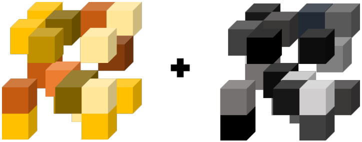
Noisy tensor completion



Mathematical model



$\boldsymbol{T}^{\star}$



$\boldsymbol{T}^{\mathsf{obs}}$

- unknown rank-r tensor $\boldsymbol{T}^{\star} \in \mathbb{R}^{d \times d \times d}$

$$\boldsymbol{T}^{\star} = \sum_{i=1}^{r} \boldsymbol{u}_i^{\star} \otimes \boldsymbol{u}_i^{\star} \otimes \boldsymbol{u}_i^{\star}$$

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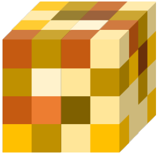

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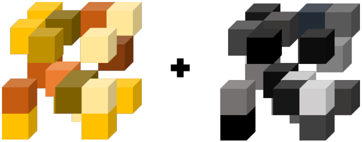

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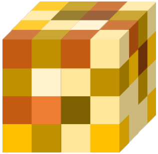
- partial observations over a sampling set Ω

$$T_{i,j,k}^{\mathsf{obs}} = T_{i,j,k}^{\star} + \text{noise}, \qquad (i,j,k) \in \Omega$$

Mathematical model



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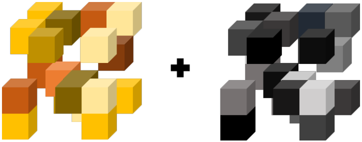

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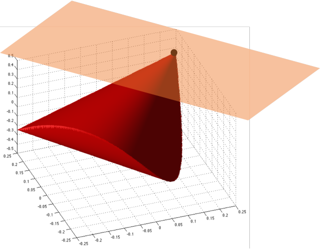
- partial observations over a sampling set Ω

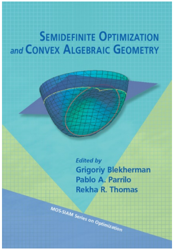
$$T_{i,j,k}^{\text{obs}} = T_{i,j,k}^{\star} + \text{noise}, \qquad (i,j,k) \in \Omega$$

- **goal:** estimate $\{\boldsymbol{u}_i^{\star}\}_{i=1}^{r}$ and $\boldsymbol{T}^{\star}$

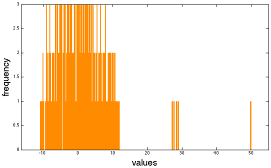
Prior art



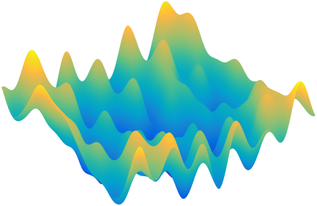
convex relaxation



sum-of-squares hierarchy



spectral methods



nonconvex optimization

Prior art

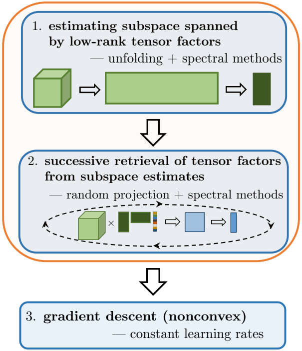
- Gandy, Recht, Yamada '11
- Liu, Musialski, Wonka, Ye '12
- Kressner, Steinlechner, Vandereycken '13
- Xu, Hao, Yin, Su '13
- Romera-Paredes, Pontil '13
- Jain, Oh '14
- Huang, Mu, Goldfarb, Wright '15
- Barak, Moitra '16
- Zhang, Aeron '16
- Yuan, Zhang '16
- Montanari, Sun '16
- Kasai, Mishra '16
- Potechin, Steurer '17
- Dong, Yuan, Zhang '17
- Xia, Yuan '19
- Zhang '19
- **Cai, Li, Poor, Chen '19**
- Cai, Li, Chi, Poor, Chen '19
- Liu, Moitra '20
- ...

A nonconvex approach: Cai et al. (NeurIPS 19)

$$\underset{\boldsymbol{U}=[\boldsymbol{u}_1,\cdots,\boldsymbol{u}_r]\in\mathbb{R}^{d\times r}}{\text{minimize}} \; f(\boldsymbol{U}) := \underbrace{\sum_{(i,j,k)\in\Omega} \Big\{ \Big(\sum\nolimits_{s=1}^{r} \boldsymbol{u}_s^{\otimes 3} \Big)_{i,j,k} - T_{i,j,k}^{\mathsf{obs}} \Big\}^2}_{\text{squared loss}}$$

- proper initializaiton: $\boldsymbol{U}^0$
- gradient descent: for $t = 0, 1, \cdots$

$$\boldsymbol{U}^{t+1} = \boldsymbol{U}^t - \eta_t \nabla f(\boldsymbol{U}^t)$$



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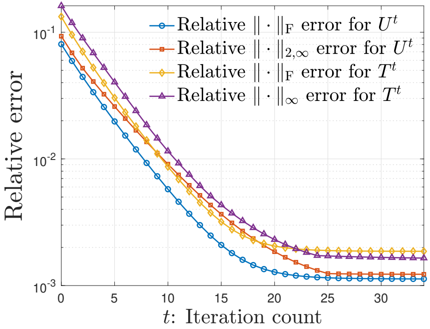
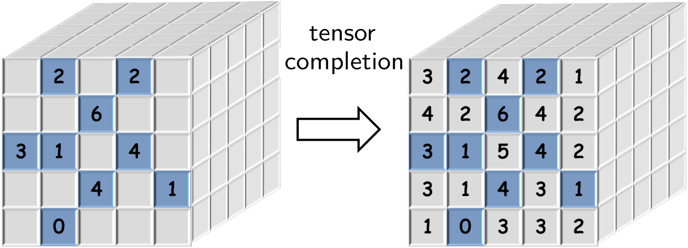


Under mild conditions, this nonconvex algorithm achieves

- linear convergence
- minimax-optimal statistical accuracy (up to log factor)

One step further: reasoning about uncertainty?



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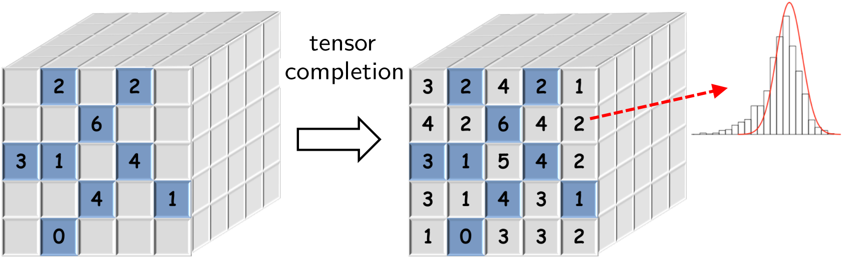

How to assess uncertainty, or "confidence", of obtained estimates due to imperfect data acquisition?

- noise
- incomplete measurements
- $\cdots$

Challenges

$$\underset{\boldsymbol{U}=[\boldsymbol{u}_1,\cdots,\boldsymbol{u}_r]\in\mathbb{R}^{d\times r}}{\text{minimize}} \; f(\boldsymbol{U}) := \underbrace{\sum_{(i,j,k)\in\Omega} \Big\{ \Big(\sum\nolimits_{s=1}^{r} \boldsymbol{u}_s^{\otimes 3} \Big)_{i,j,k} - T_{i,j,k}^{\mathsf{obs}} \Big\}^2}_{\text{squared loss}}$$

- how to pin down distributions of nonconvex solutions?

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- how to pin down distributions of nonconvex solutions?
- how to adapt to unknown noise distributions and heteroscedasticity (i.e. location-varying noise variance)?

Challenges

$$\underset{\boldsymbol{U}=[\boldsymbol{u}_1,\cdots,\boldsymbol{u}_r]\in\mathbb{R}^{d\times r}}{\text{minimize}} \; f(\boldsymbol{U}) := \underbrace{\sum_{(i,j,k)\in\Omega} \Big\{ \Big(\sum\nolimits_{s=1}^{r} \boldsymbol{u}_s^{\otimes 3} \Big)_{i,j,k} - T_{i,j,k}^{\mathsf{obs}} \Big\}^2}_{\text{squared loss}}$$

- how to pin down distributions of nonconvex solutions?
- how to adapt to unknown noise distributions and heteroscedasticity (i.e. location-varying noise variance)?
- existing estimation guarantees are highly insufficient
  $\longrightarrow$ overly wide confidence intervals

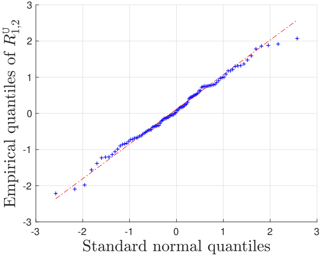
Assumptions

$$\boldsymbol{T}^\star = \sum_{i=1}^{r} \boldsymbol{u}_i^\star \otimes \boldsymbol{u}_i^\star \otimes \boldsymbol{u}_i^\star \in \mathbb{R}^{d\times d\times d}$$

- **random sampling**: each entry is observed independently with prob. $p \gtrsim \frac{\mathrm{polylog}(d)}{d^{3/2}}$
- **random noise**: independent zero-mean sub-Gaussian with variance of roughly the same order (but not identical)
- **ground truth**: low-rank ($r = O(1)$), incoherent (tensor factors are de-localized and nearly orthogonal to each other), and well-conditioned

Main results: distributional theory

- random sampling
- independent sub-Gaussian noise
- ground truth: low-rank, incoherent, well-conditioned



Theorem 1

With high prob., there exists permutation matrix $\mathbf{\Pi} \in \mathbb{R}^{r \times r}$ s.t.

$$\boldsymbol{U}\mathbf{\Pi} - \boldsymbol{U}^{\star} \sim \mathcal{N}(\mathbf{0}, \textit{Cramér-Rao}) + \textit{negligible term}$$

— *asymptotically optimal*

Main results: distributional theory

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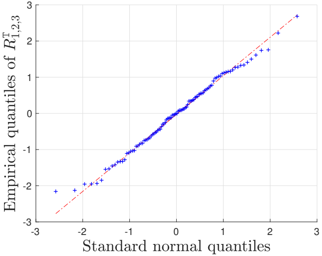


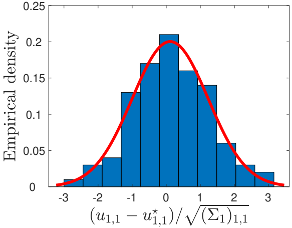
Theorem 2

Consider any (i, j, k) s.t. the corresponding "SNR" is not exceedingly small. Then with high prob.,

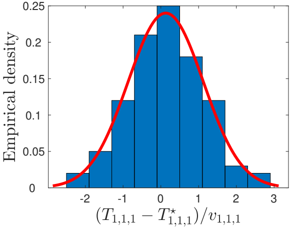
$$T_{i,j,k} - T^{\star}_{i,j,k} \sim \mathcal{N}(0, \textit{Cramér-Rao}) + \textit{negligible term}$$

— *asymptotically optimal*

- **Gaussianality and optimality:** estimation error of nonconvex approach is zero-mean Gaussian, who (co)-variance is “minimal”

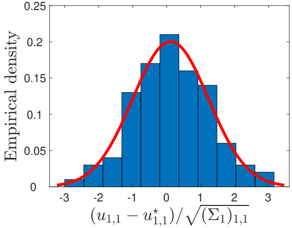


tensor factor entry



tensor entry

- **Gaussianality and optimality:** estimation error of nonconvex approach is zero-mean Gaussian, who (co)-variance is "minimal"
- **Confidence intervals:** error (co)-variance can be accurately estimated, leading to valid CI construction



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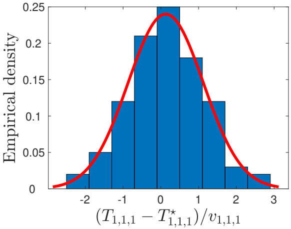

tensor entry

- **Gaussianality and optimality:** estimation error of nonconvex approach is zero-mean Gaussian, who (co)-variance is "minimal"
- **Confidence intervals:** error (co)-variance can be accurately estimated, leading to valid CI construction
- **Adaptivity:** our procedure is data-driven, fully adaptive to unknown noise levels and heteroscedasticity

Empirical coverage rates (CR)

tensor factor

(r,σ)	Mean(CR)	Std(CR)
$(2,10^{-2})$	0.9481	0.0201
$(2,10^{-1})$	0.9477	0.0228
$(2,1)$	0.9478	0.0215
$(4,10^{-2})$	0.9450	0.0218
$(4,10^{-1})$	0.9472	0.0231
$(4,1)$	0.9462	0.0234

tensor entries

(r,σ)	Mean(CR)	Std(CR)
$(2,10^{-2})$	0.9494	0.0218
$(2,10^{-1})$	0.9513	0.0218
$(2,1)$	0.9475	0.0222
$(4,10^{-2})$	0.9434	0.0225
$(4,10^{-1})$	0.9494	0.0220
$(4,1)$	0.9494	0.0219

$d=100,\ p=0.2,$ heteroscedastic

Back to estimation: ℓ_2 optimality

Distributional theory in turn allows us to track estimation accuracy

Back to estimation: ℓ_2 optimality

Distributional theory in turn allows us to track estimation accuracy

Theorem 3

Suppose noise is i.i.d. Gaussian. $\exists$ *some permutation* $\pi(\cdot)$ *s.t.*

$$\|\boldsymbol{u}_{\pi(l)} - \boldsymbol{u}_l^\star\|_2^2 = \underbrace{\frac{(2+o(1))\sigma^2 d}{p\|\boldsymbol{u}_l^\star\|_2^4}}_{\text{Cram er-Rao lower bound}}, \quad 1 \le l \le r$$

$$\|\boldsymbol{T} - \boldsymbol{T}^\star\|_{\mathrm{F}}^2 = \underbrace{\frac{(6+o(1))\sigma^2 rd}{p}}_{\text{Cramér-Rao lower bound}}$$

Back to estimation: ℓ_2 optimality

Distributional theory in turn allows us to track estimation accuracy

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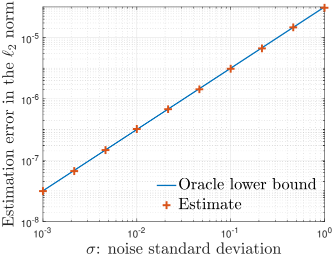
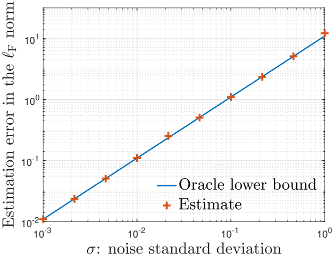
$$\|\boldsymbol{T} - \boldsymbol{T}^\star\|_{\mathrm{F}}^2 = \underbrace{\frac{(6+o(1))\sigma^2 r d}{p}}_{\text{Cramér-Rao lower bound}}$$

- precise characterization of estimation accuracy
- achieves full statistical efficiency (including pre-constant)

Numerical ℓ_2 errors vs. Cramér–Rao bounds



tensor factor estimation



tensor estimation

$$r = 4,\ p = 0.2,\ d = 100$$

Concluding remarks

nonconvex optimization

optimal estimation guarantees

fast, adaptive to unknown noise levels

optimal uncertainty quantification

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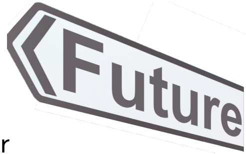

future directions

- improve dependency on rank & cond. number
- more general sampling patterns
- other tensor-type problems

Paper:

"Uncertainty quantification for nonconvex tensor completion: Confidence intervals, heteroscedasticity and optimality," C. Cai, H. V. Poor, Y. Chen, ICML 2020

Other related papers:

"Nonconvex low-rank symmetric tensor completion from noisy data," C. Cai, G. Li, H. V. Poor, Y. Chen, NeurIPS 2019

"Subspace estimation from unbalanced and incomplete data matrices: $\ell_{2,\infty}$ statistical guarantees," C. Cai, G. Li, Y. Chi, H. V. Poor, Y. Chen, accepted to Annals of Statistics, 2019