Towards better computation-statistics trade-off in tensor decomposition

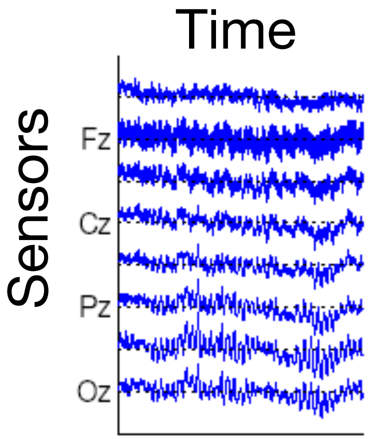
Ryota Tomioka
TTI Chicago

Joint work with: T. Suzuki, K. Hayashi, & H. Kashima

Matrices and Tensors in machine learning

Matrices

Multivariate time-series



Collaborative filtering

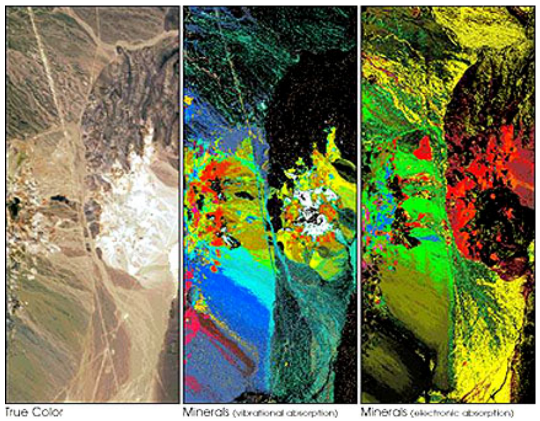
Movies

Users

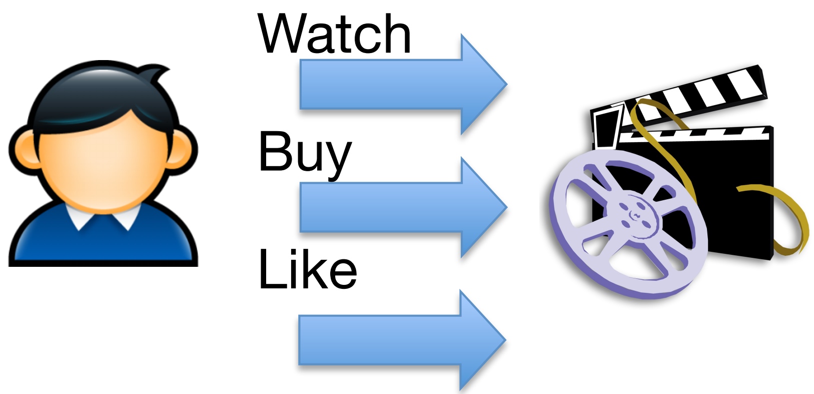
	Star Wars	Titanic	Blade Runner
User 1	5	2	4
User 2	1	4	2
User 3	5	?	?

Tensors

Spatio-temoral data



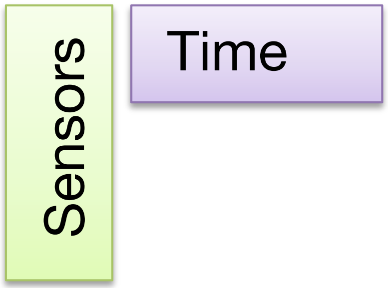
Multiple relations



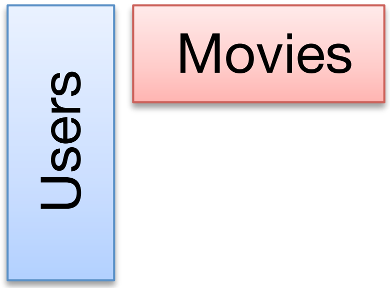
Matrices and Tensors in machine learning

Matrices

Multivariate time-series

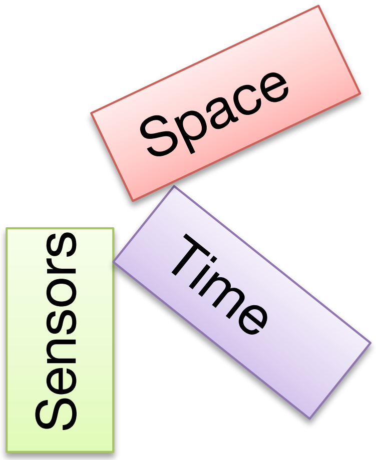


Collaborative filtering

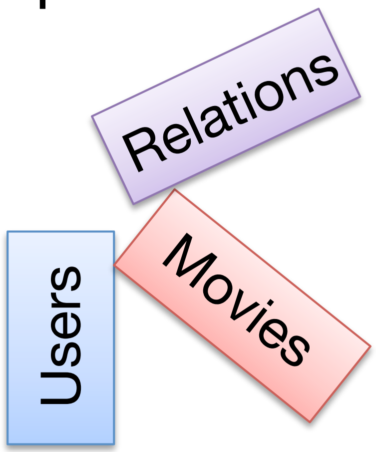


Tensors

Spatio-temoral data



Multiple relations



From matrices to tensors

- Trace norm: convex relaxation of matrix rank

$$\|\boldsymbol{W}\|_{S_1} = \sum_{j=1}^{r} \sigma_j(\boldsymbol{W})$$

Induces low-rank-ness (spectral sparsity)

  - It works like L1 regularization on the singular values
  - Performance guarantees [Srebro & Schraibman 2005; Candes & Recht 2009; Candes & Tao 2010; Negahban & Wainwright 2011]

Similar relaxation possible for tensor rank?

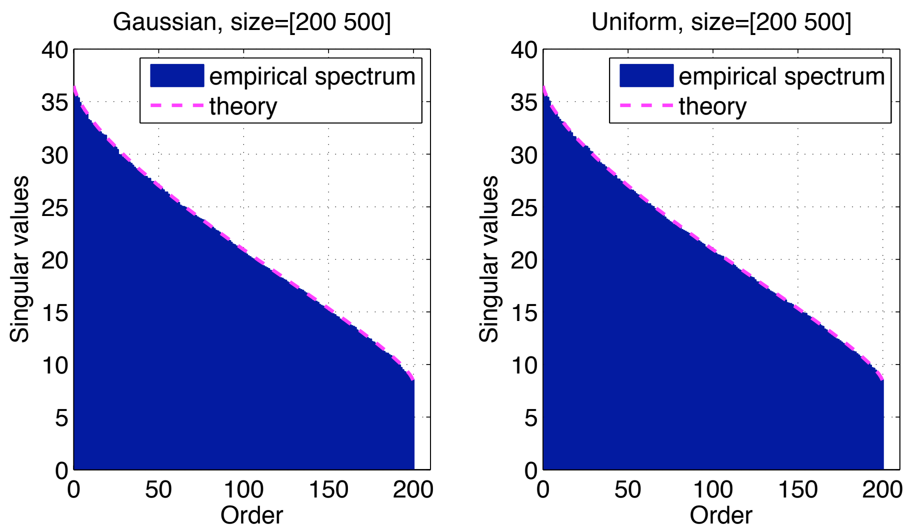
From matrices to tensors

- Spectral norm of random Gaussian matrix

$$\mathbb{E}\|\boldsymbol{X}\|_{S_\infty} \leq \sigma\left(\sqrt{m}+\sqrt{n}\right)$$

- Marchenko-Pastur distribution

[Marchenko & Pastur 1967]



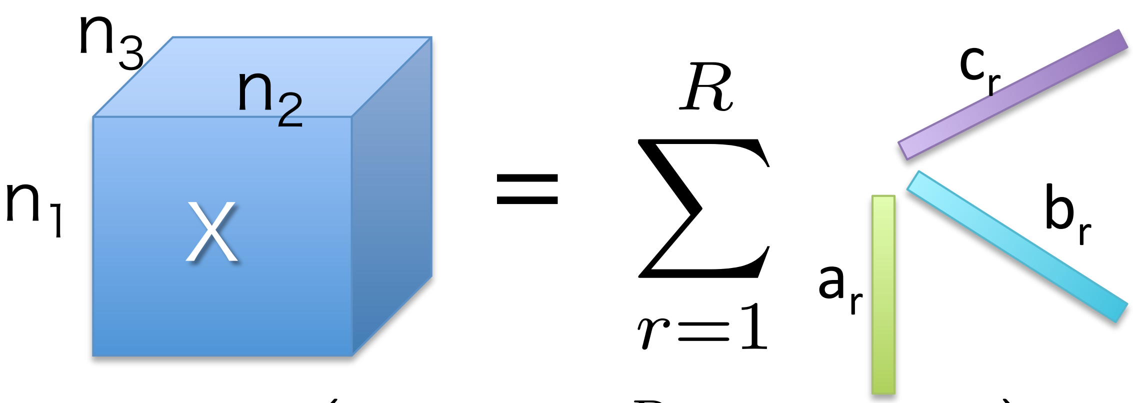
Random *tensor* theory?

Outline

- Tensor ranks and decompositions
- Overlapped trace norm (moderate computation)
  - Limitations: requires $O(rn^{K-1})$ samples
- Balanced trace norm (heavy computation) [Mu et al. 2013]
  - requires $O(r^{K/2}n^{K/2})$ samples
- Tensor trace norm (probably intractable)
  - requires only $O(rn)$ samples

Tensor rank

- Minimum number R such that



$$\left(X_{ijk} = \sum_{r=1}^{R} a_{ir} b_{jr} c_{kr} \right)$$

(for 3rd order tensor)

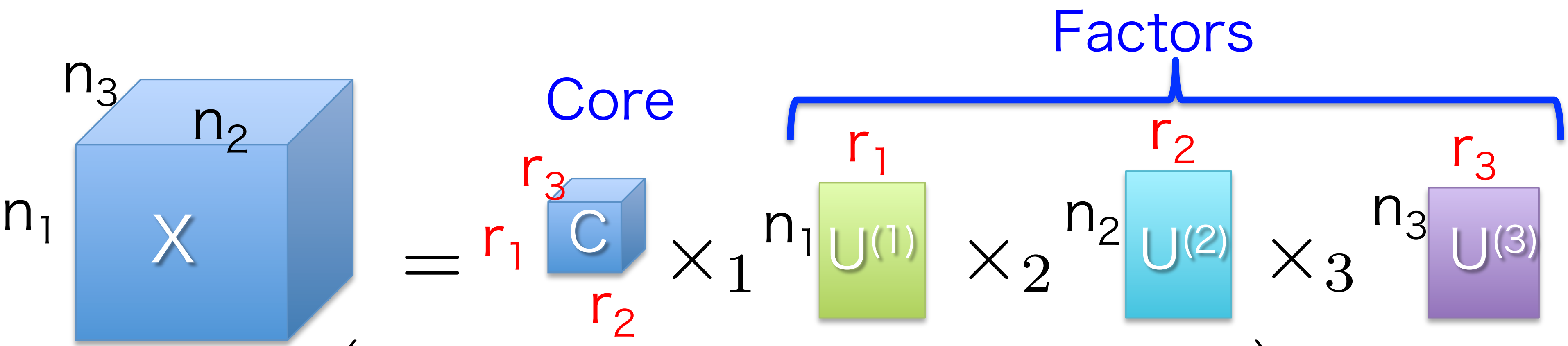
- Known as CP (canonical polyadic) decomposition

[Hitchcock 27; Carroll & Chang 70; Harshman 70]

- Comutation of the above decomposition is NP hard!

Tucker decomposition

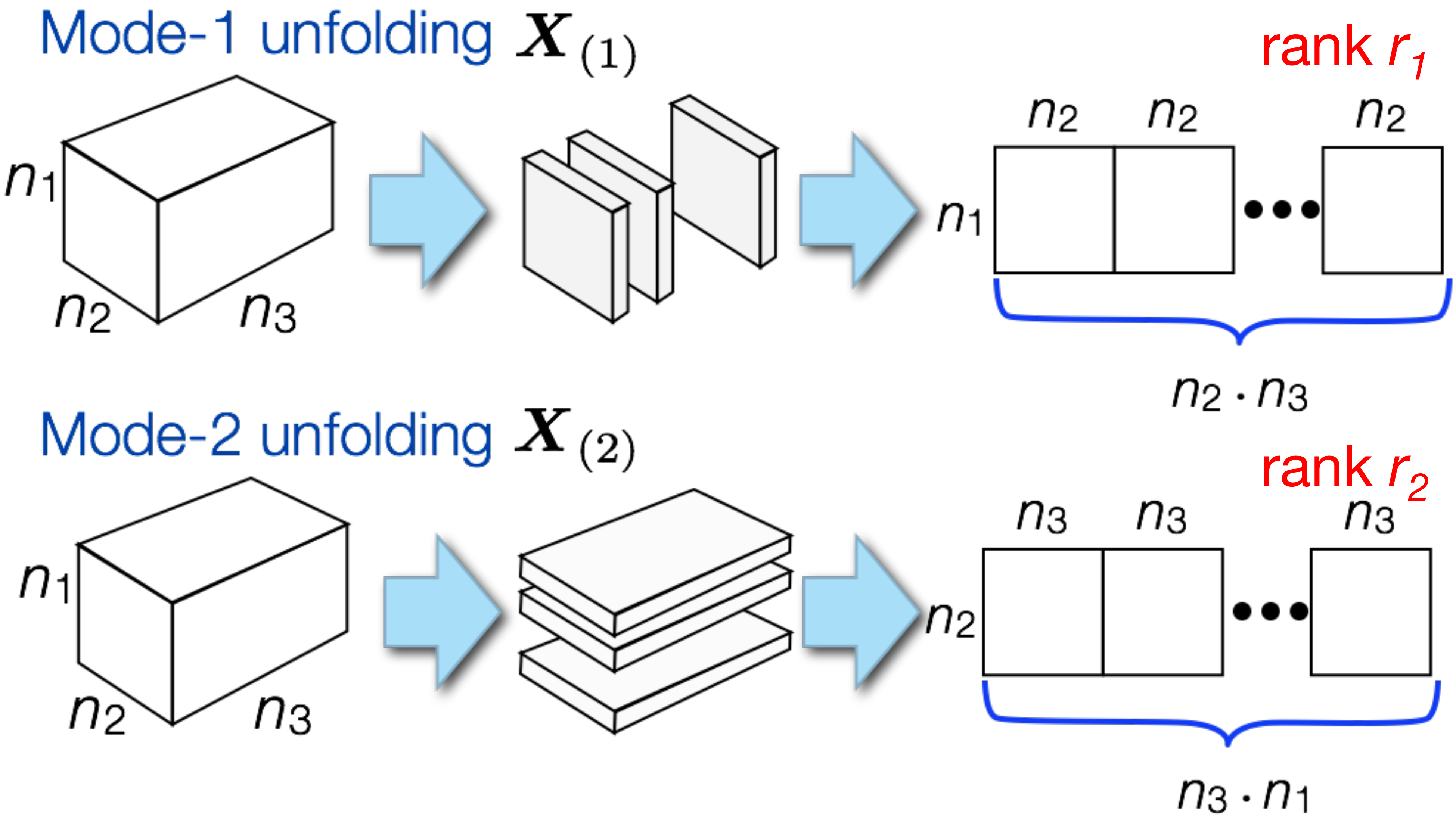
[Tucker 66; De Lathauwer+00]



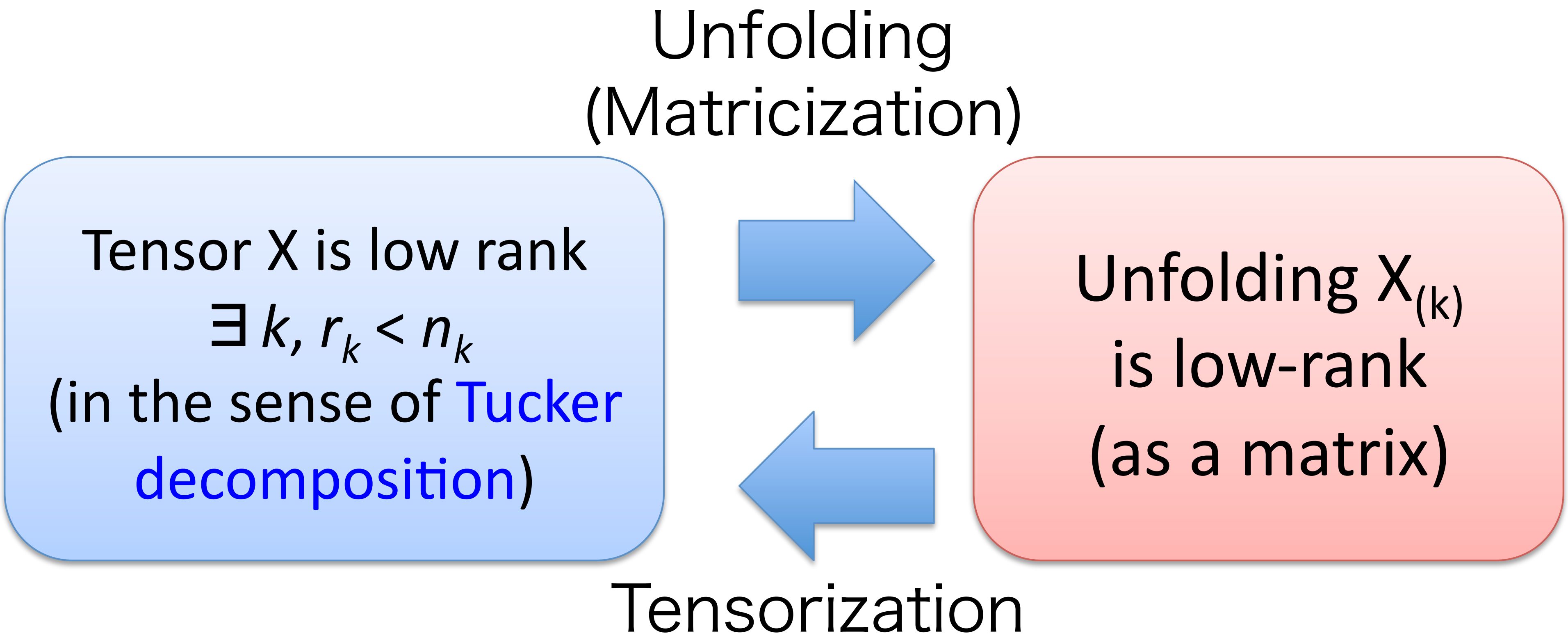
$$\left(X_{ijk} = \sum_{a=1}^{r_1} \sum_{b=1}^{r_2} \sum_{c=1}^{r_3} C_{abc} U_{ia}^{(1)} U_{jb}^{(2)} U_{kc}^{(3)} \right)$$

- Factors can be obtained by unfolding operation+SVD
- In practice no unfolding is low-rank --- Common solution: iterate truncated SVD (HOSVD, HOOI); non-convex

Unfolding (matricization)



Core idea


Unfolding
(Matricization)
Tensor X is low rank
$\exists\, k, r_k < n_k$
(in the sense of Tucker decomposition)
Unfolding $X_{(k)}$
is low-rank
(as a matrix)
Tensorization

Overlapped trace norm

[T+10; Signoretto+10; Gandy+11; Liu+09]

- Convex optimization problem

$$\underset{\mathcal{W}\in\mathbb{R}^{n_1\times\cdots\times n_K}}{\text{minimize}} \quad \frac{1}{2}\|\boldsymbol{y}-\mathfrak{X}(\mathcal{W})\|^2+\lambda_M|||\mathcal{W}|||_{\underline{S_1/1}}$$

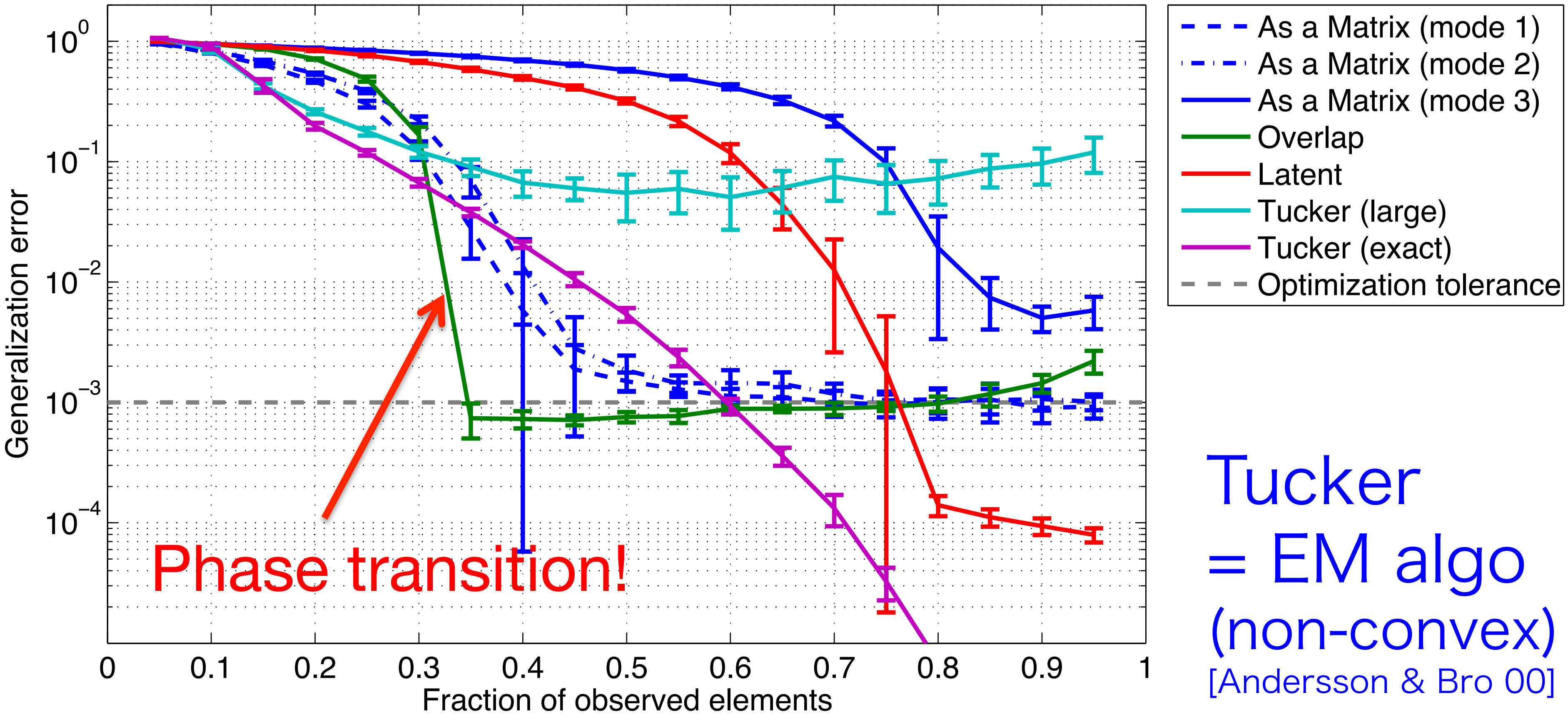
where $\quad |||\mathcal{W}|||_{\underline{S_1/1}} := \sum_{k=1}^{K}\|\boldsymbol{W}_{(k)}\|_{S_1}$

mode-*k* unfolding

– the same tensor is regularized to be simultaneously low-rank w.r.t. all modes.

Empirical performance

- True tensor: 50x50x20, rank 7x8x9. No noise (λ=0).
- Random train/test split.



Tucker
= EM algo
(non-convex)
[Andersson & Bro 00]

Analysis: Problem setting

Observation

$\mathcal{W}^*$: true tensor with rank ($r_1,\ldots,r_K$)

$$y_i = \langle \mathcal{X}_i, \mathcal{W}^* \rangle + \epsilon_i \quad (i = 1, \ldots, M)$$

Gaussian noise $N(0,\sigma^2)$

Optimization

Likelihood Regularization

$$\hat{\mathcal{W}} = \operatorname*{argmin}_{\mathcal{W} \in \mathbb{R}^{n_1 \times \cdots \times n_K}} \left(\frac{1}{2} \|\boldsymbol{y} - \mathfrak{X}(\mathcal{W})\|^2 + \lambda_M |||\mathcal{W}|||_{\underline{S_1/1}} \right)$$

Reg. constant

$$(N = \textstyle\prod_{k=1}^{K} n_k)$$

Observation operator $\mathfrak{X} : \mathbb{R}^N \to \mathbb{R}^M$

$$\mathfrak{X}(\boldsymbol{\mathcal{W}}) = (\langle \boldsymbol{\mathcal{X}}_1, \boldsymbol{\mathcal{W}} \rangle, \ldots, \langle \boldsymbol{\mathcal{X}}_M, \boldsymbol{\mathcal{W}} \rangle)^\top$$

Theorem ("overlapped" approach)

[T, Suzuki, Hayashi, Kashima 11]

Assume that the elements of the design X are independently and identically Gaussian distributed. Moreover, if

$$\frac{\#\text{samples } (M)}{\#\text{variables } (N)} \geq c_1 \underbrace{\|\boldsymbol{n}^{-1}\|_{1/2}\|\boldsymbol{r}\|_{1/2}}_{\text{normalized rank}} \approx \frac{r}{n}$$

$$\|\boldsymbol{n}^{-1}\|_{1/2} := \left(\frac{1}{K}\sum_{k=1}^{K}\sqrt{1/n_k}\right)^2, \quad \|\boldsymbol{r}\|_{1/2} := \left(\frac{1}{K}\sum_{k=1}^{K}\sqrt{r_k}\right)^2$$

Theorem (random Gauss design)

[T, Suzuki, Hayashi, Kashima 11]

Assume that the elements of the design X are independently and identically Gaussian distributed. Moreover, if

$$\frac{\#\text{samples } (M)}{\#\text{variables } (N)} \geq c_1 \underbrace{\|\boldsymbol{n}^{-1}\|_{1/2} \|\boldsymbol{r}\|_{1/2}}_{\text{normalized rank}} \approx \frac{r}{n}$$

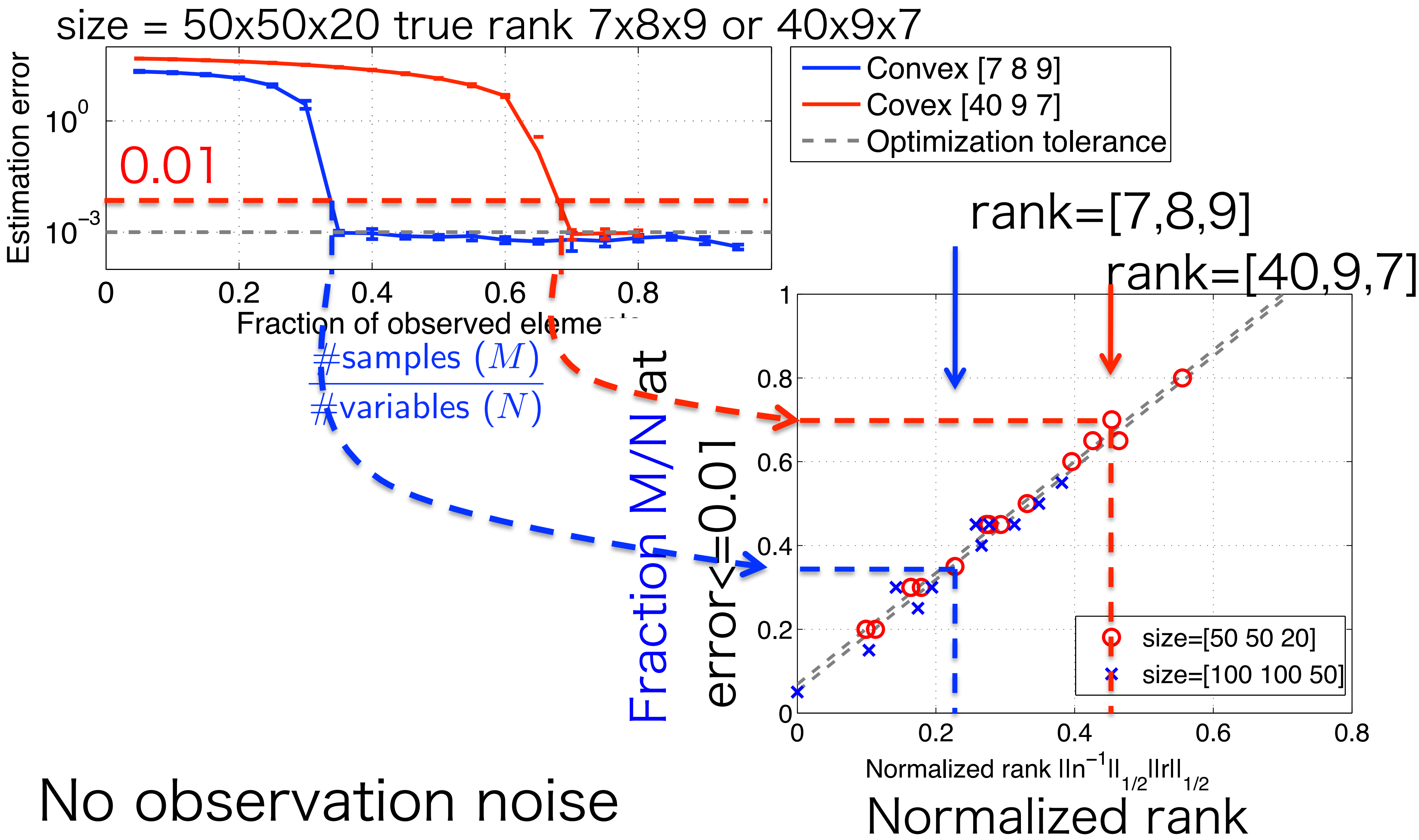
Convergence!

$$\frac{\left\| \hat{\mathcal{W}} - \mathcal{W}^* \right\|_F^2}{N} \leq O_p \left(\frac{\sigma^2 \|\boldsymbol{n}^{-1}\|_{1/2} \|\boldsymbol{r}\|_{1/2}}{M} \right)$$

(with appropriate choice of λ_M)

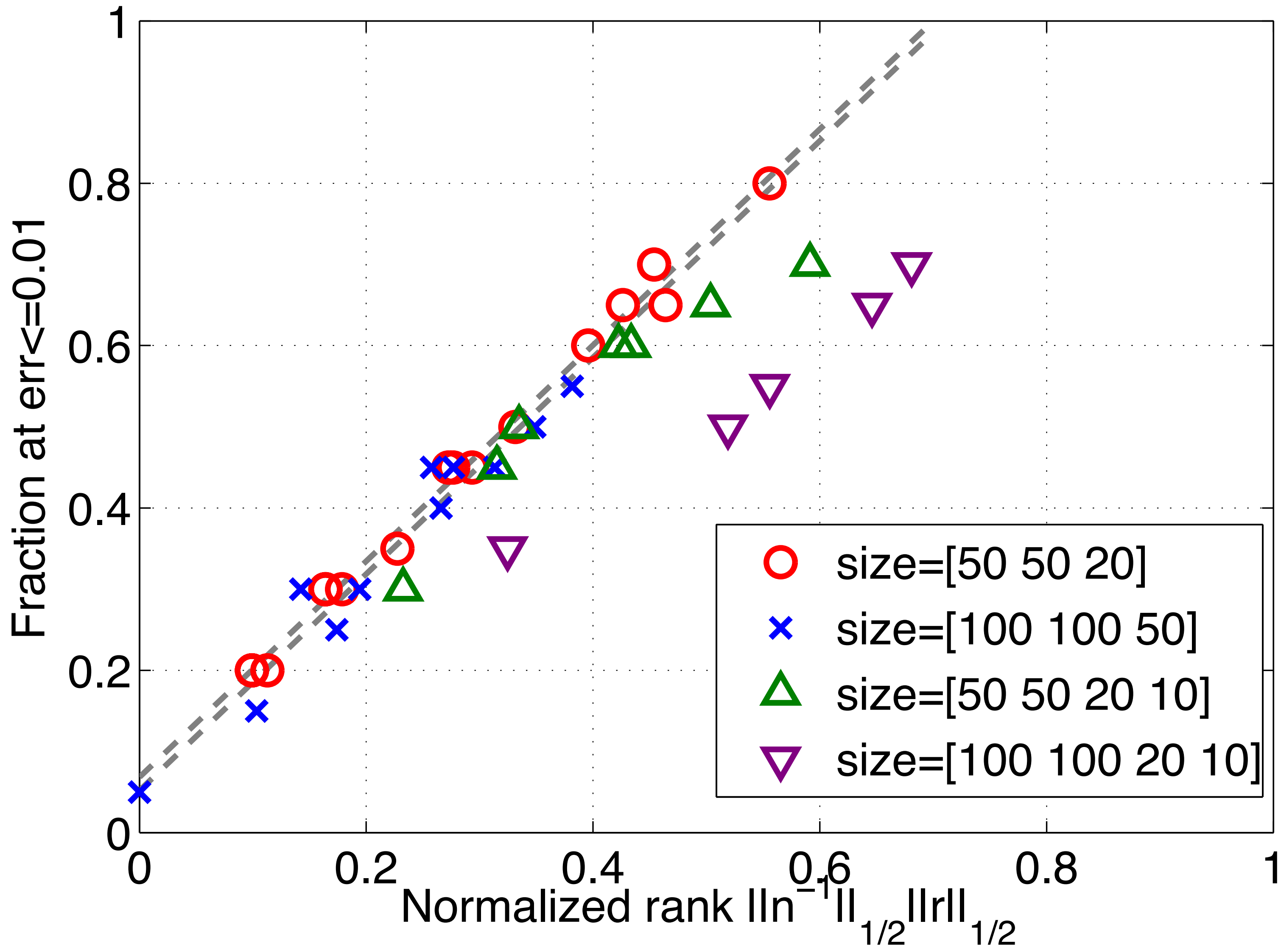
$$\|\boldsymbol{n}^{-1}\|_{1/2} := \left(\frac{1}{K} \sum_{k=1}^{K} \sqrt{1/n_k} \right)^2, \quad \|\boldsymbol{r}\|_{1/2} := \left(\frac{1}{K} \sum_{k=1}^{K} \sqrt{r_k} \right)^2$$

Tensor completion



No observation noise

Theory vs. Experiments (4th order)



Limitation: exponentially many samples required!

- Simplify by setting $n_k = n$ and $r_k = r$
- Then there are constants c0, c1, c2 such that
  - #samples $M \geq c_1 n^{K-1} r$
  - reg. const. $\lambda_M = c_0 \sigma \sqrt{n^{K-1}/M}$

$$|||\hat{\mathcal{W}} - \mathcal{W}^*|||_F^2 \leq c_2 \frac{\sigma^2 r n^{K-1}}{M}$$

with high probability.

Why?

- Key steps in the analysis
  - Relation between the norm and the rank

$$\left|\!\left|\!\left|\mathcal{W}\right|\!\right|\!\right|_{\underline{S_1/1}} \le K\sqrt{r}\left|\!\left|\!\left|\mathcal{W}\right|\!\right|\!\right|_F \qquad \text{(OK)}$$

  - Dual norm of noise tensor

$$\mathbb{E}\left|\!\left|\!\left|\mathfrak{X}^\top(\boldsymbol{\epsilon})\right|\!\right|\!\right|_{(\underline{S_1/1})^*} \le \frac{\sigma\sqrt{M}}{K}\left(\sqrt{n^{K-1}} + \sqrt{n}\right)$$

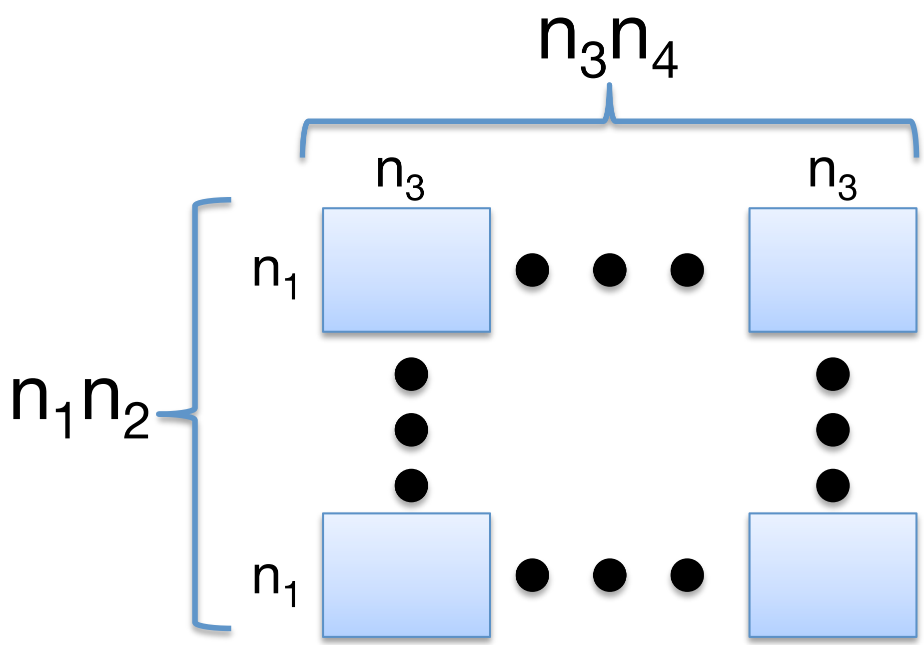
unbalanced (Bad)

where $\mathfrak{X}^\top(\boldsymbol{\epsilon}) := \sum_{i=1}^{M} \epsilon_i \mathcal{X}_i$

Balanced unfolding

- For K>3, there are 2^{K-1}-1 > K ways to unfold a tensor. For example,

$$\boldsymbol{X}_{(1,2;3,4)} =$$



(See also Mu et al. 2013)

Balanced trace norm (for K=4)

- Definition

$$|||\mathcal{W}|||_{\text{balanced}} := \|\boldsymbol{W}_{(1,2;3,4)}\|_{S_1} + \|\boldsymbol{W}_{(1,3;2,4)}\|_{S_1} + \|\boldsymbol{W}_{(1,4;2,3)}\|_{S_1}$$

– Relation between the norm and the rank

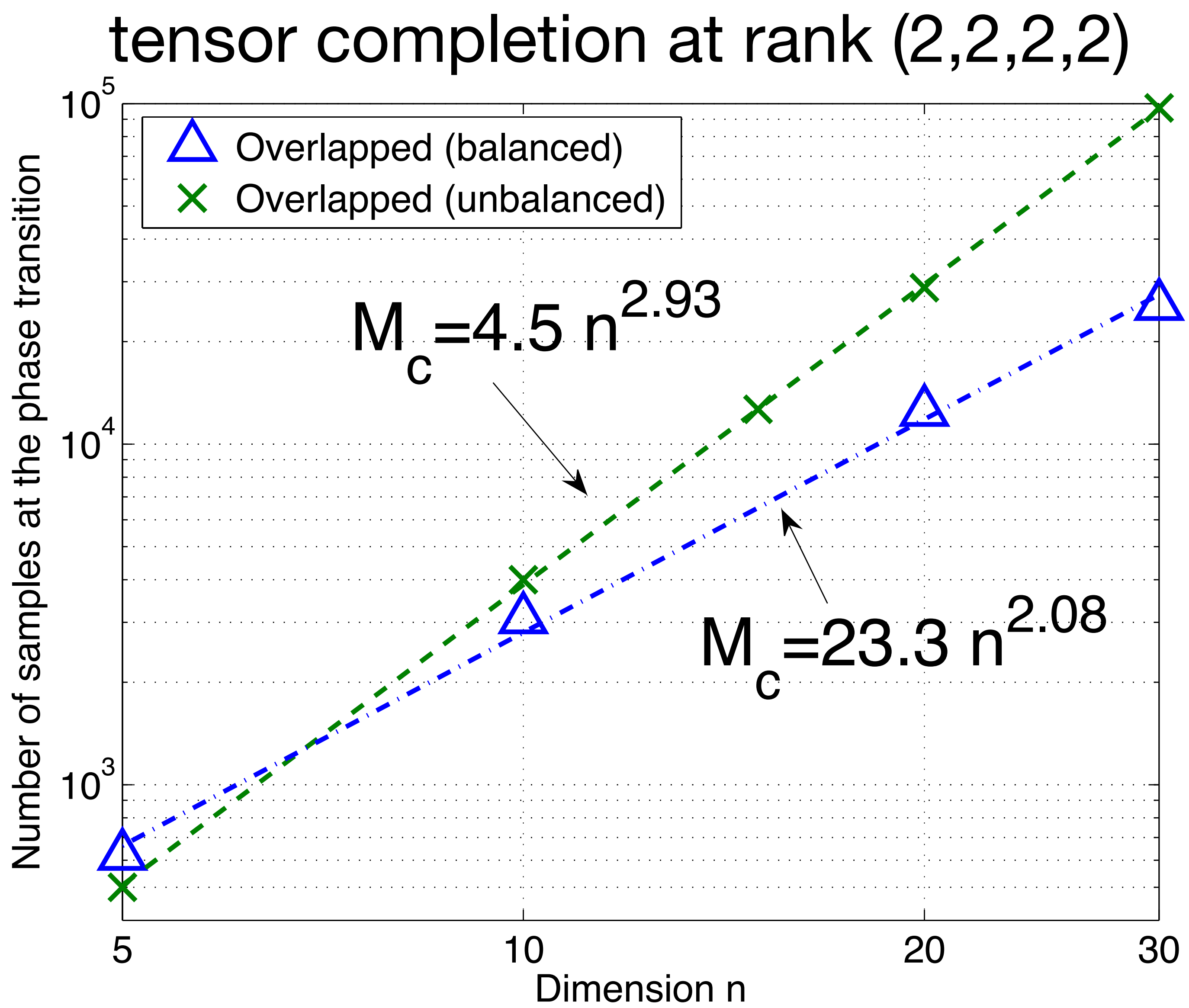
$$|||\mathcal{W}|||_{\text{balanced}} \leq 3\sqrt{r^2}\,|||\mathcal{W}|||_F$$

– Dual norm of noise tensor

$$\mathbb{E}|||\mathfrak{X}^\top(\boldsymbol{\epsilon})|||_{\text{balanced}^*} \leq \frac{\sigma\sqrt{M}}{3} \cdot 2\sqrt{n^2}$$

Sample complexity $O(r^2 n^2)$

Experiment (K=4)



Theoretically

× $O(n^3)$

△ $O(n^2)$

Comparison of computational complexity

- Overlapped trace norm (Sample Complex. $O(rn^{K-1})$)
  - requires SVD of n^{K-1} x n matrix: Large!

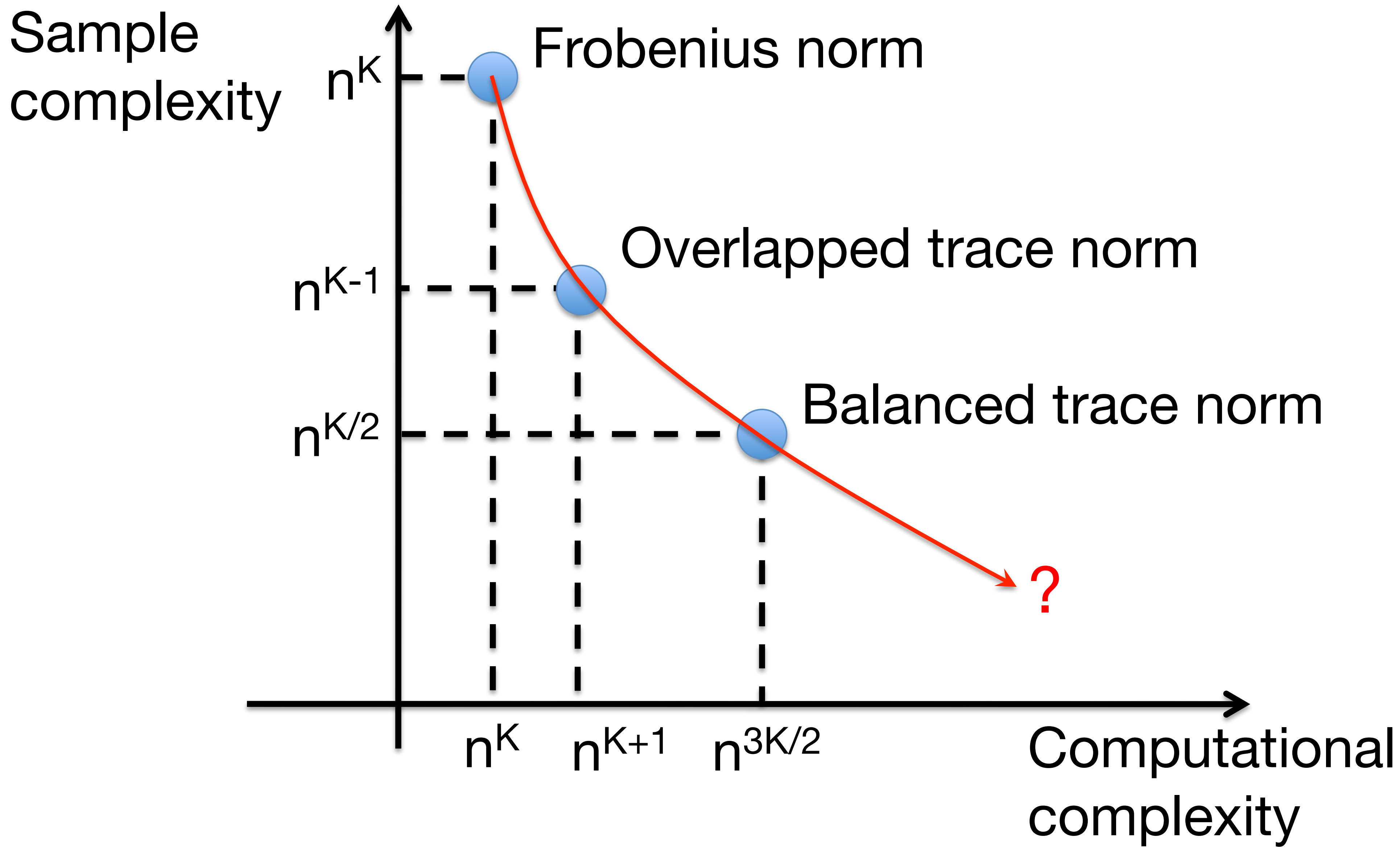
    $O(n^{K+1}+n^3)$ ⇒ $O(n^5)$ for K=4 OK

- Balanced trace norm (Sample Complex. $O(r^{K/2}n^{K/2})$)
  - requires SVD of $n^{K/2}$ x $n^{K/2}$ matrix: OK

    $O(n^{1.5K})$ ⇒ $O(n^6)$ for K=4 Large!

statistically more efficient, computationally more challenging!

Computation-statistics trade-off



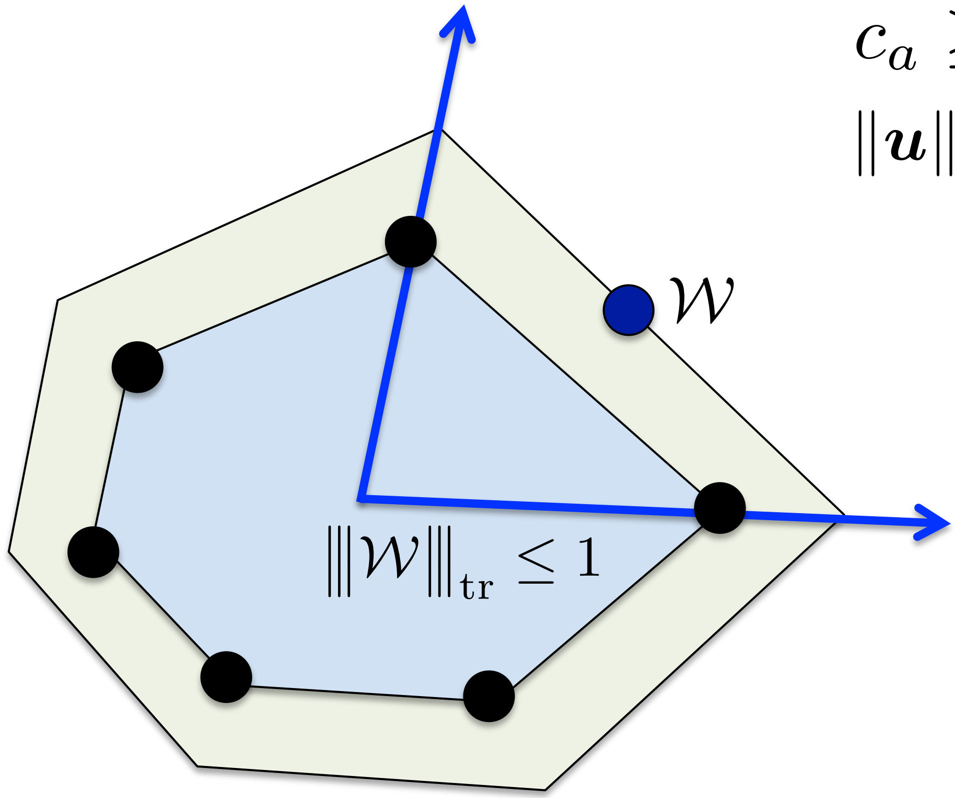
Tensor trace norm

For K=3

$$\|\mathcal{W}\|_{\mathrm{tr}} = \inf \sum_{a \in \mathcal{A}} c_a \quad \text{s.t.} \quad \mathcal{W} = \sum_{a \in \mathcal{A}} c_a \boldsymbol{u}_a \circ \boldsymbol{v}_a \circ \boldsymbol{w}_a$$

$$c_a \geq 0$$

$$\|\boldsymbol{u}\| \leq 1,\ \|\boldsymbol{v}\| \leq 1,\ \|\boldsymbol{w}\| \leq 1$$



rank-1 tensor (outer prod. of vectors)

can be seen as an atomic norm [Chandrasekaran 12] with atomic set = set of rank-1 tensors

Tensor trace norm

For K=3

$$\|\!|\mathcal{W}|\!\|_{\mathrm{tr}} = \inf \sum_{a\in\mathcal{A}} c_a \quad \text{s.t.} \quad \mathcal{W} = \sum_{a\in\mathcal{A}} c_a \boldsymbol{u}_a \circ \boldsymbol{v}_a \circ \boldsymbol{w}_a$$

$$c_a \geq 0$$

$$\|\boldsymbol{u}\| \leq 1,\ \|\boldsymbol{v}\| \leq 1,\ \|\boldsymbol{w}\| \leq 1$$

Relation between the norm and the orthogonal CP rank

(Kolda 2001)

$$\|\!|\mathcal{W}|\!\|_{\mathrm{tr}} \leq \sqrt{R}\,\|\!|\mathcal{W}|\!\|_{F}$$

Dual norm of the noise tensor

$$\mathbb{E}\|\!|\mathfrak{X}^{\top}(\boldsymbol{\epsilon})|\!\|_{\mathrm{tr}^*} \leq C\sigma\sqrt{M}\sqrt{n}$$

⇨ Sample complexity O(Rn)

Dual of the trace norm is the *tensor operator norm*

$$\left\|\!\left|\mathcal{Y}\right|\!\right\|_{\mathrm{tr}^*} = \left\|\!\left|\mathcal{Y}\right|\!\right\|_{\mathrm{op}} := \sup_{\boldsymbol{u},\boldsymbol{v},\boldsymbol{w}} \sum_{i,j,k} Y_{ijk} u_i v_j w_k$$

$$\text{s.t. } \|\boldsymbol{u}\| \leq 1,\ \|\boldsymbol{v}\| \leq 1,\ \|\boldsymbol{w}\| \leq 1$$

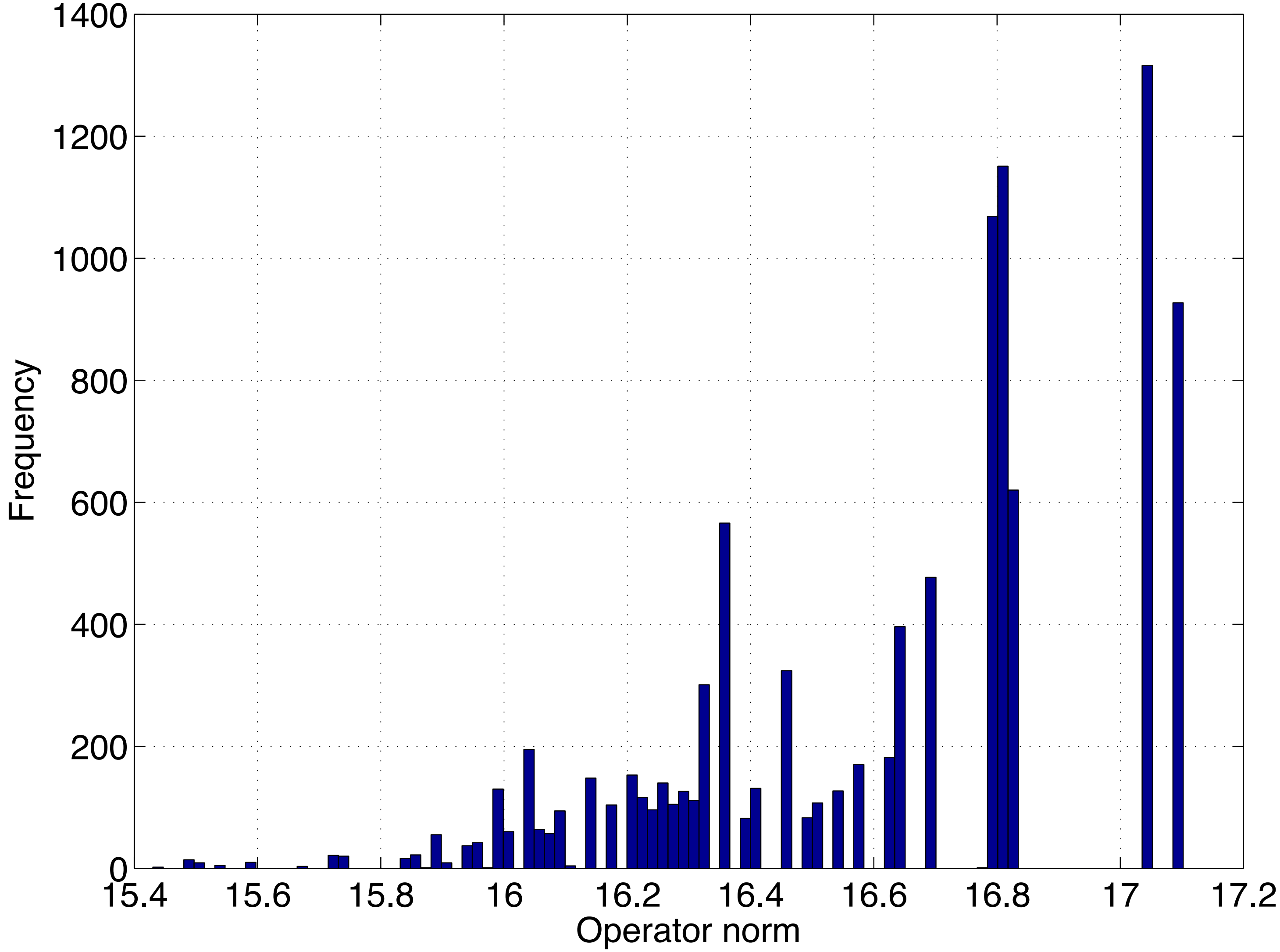
Greedy algorithm for computing the operator norm

1. Initialize u, v, w.
2. Fix u, maximize over v and w (matrix operator norm)
3. Cycle over v, w, u, … until convergence

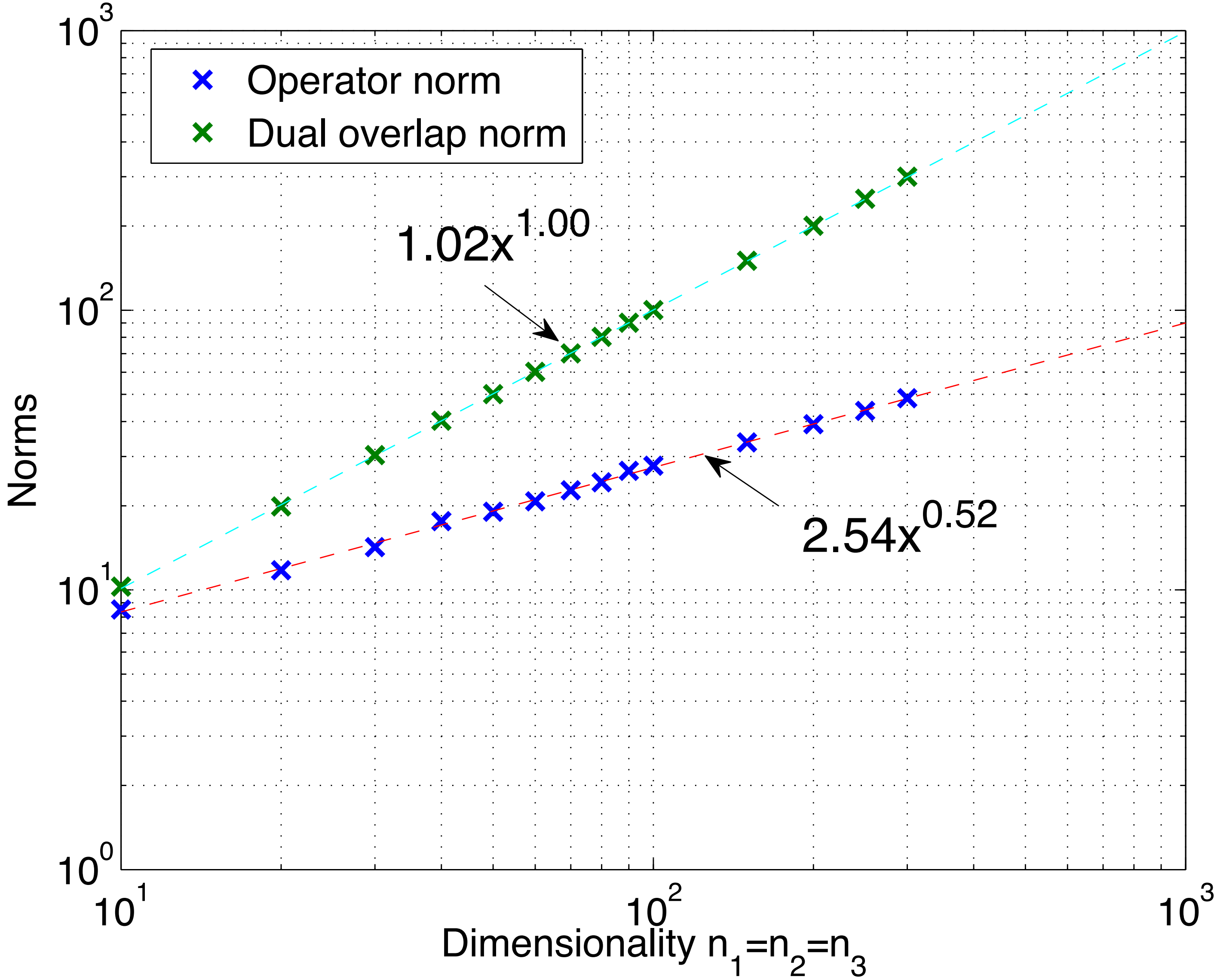
(can be improved by incorporating gradient)

10,000 random restarts

Operator norm of a random 50x50x20 tensor



Empirical scaling (K=3)



Theoretically
× O(n)
x O(√n)

Low-rank tensor estimation with the *tensor trace norm*

Likelihood — Regularization

$$\underset{\mathcal{W}\in\mathbb{R}^{n_1\times\cdots\times n_K}}{\text{minimize}} \quad \frac{1}{2}\|\boldsymbol{y}-\mathfrak{X}(\mathcal{W})\|^2 + \lambda_M |||\mathcal{W}|||_{\mathrm{tr}}$$

Key operation: prox operator

$$\mathrm{prox}_\lambda(\mathcal{W}) = \underset{\mathcal{Y}}{\mathrm{argmin}}\left(\lambda|||\mathcal{Y}|||_{\mathrm{tr}} + \frac{1}{2}|||\mathcal{Y}-\mathcal{W}|||_F^2\right)$$

$$= \mathcal{W} - \mathrm{proj}_\lambda(\mathcal{W}) \quad \text{(Moreau's theorem)}$$

$$\mathrm{proj}_\lambda(\mathcal{W}) = \underset{\mathcal{Y}}{\mathrm{argmin}}|||\mathcal{W}-\mathcal{Y}|||_F \quad \text{s.t.} \quad |||\mathcal{Y}|||_{\mathrm{op}} \le \lambda$$

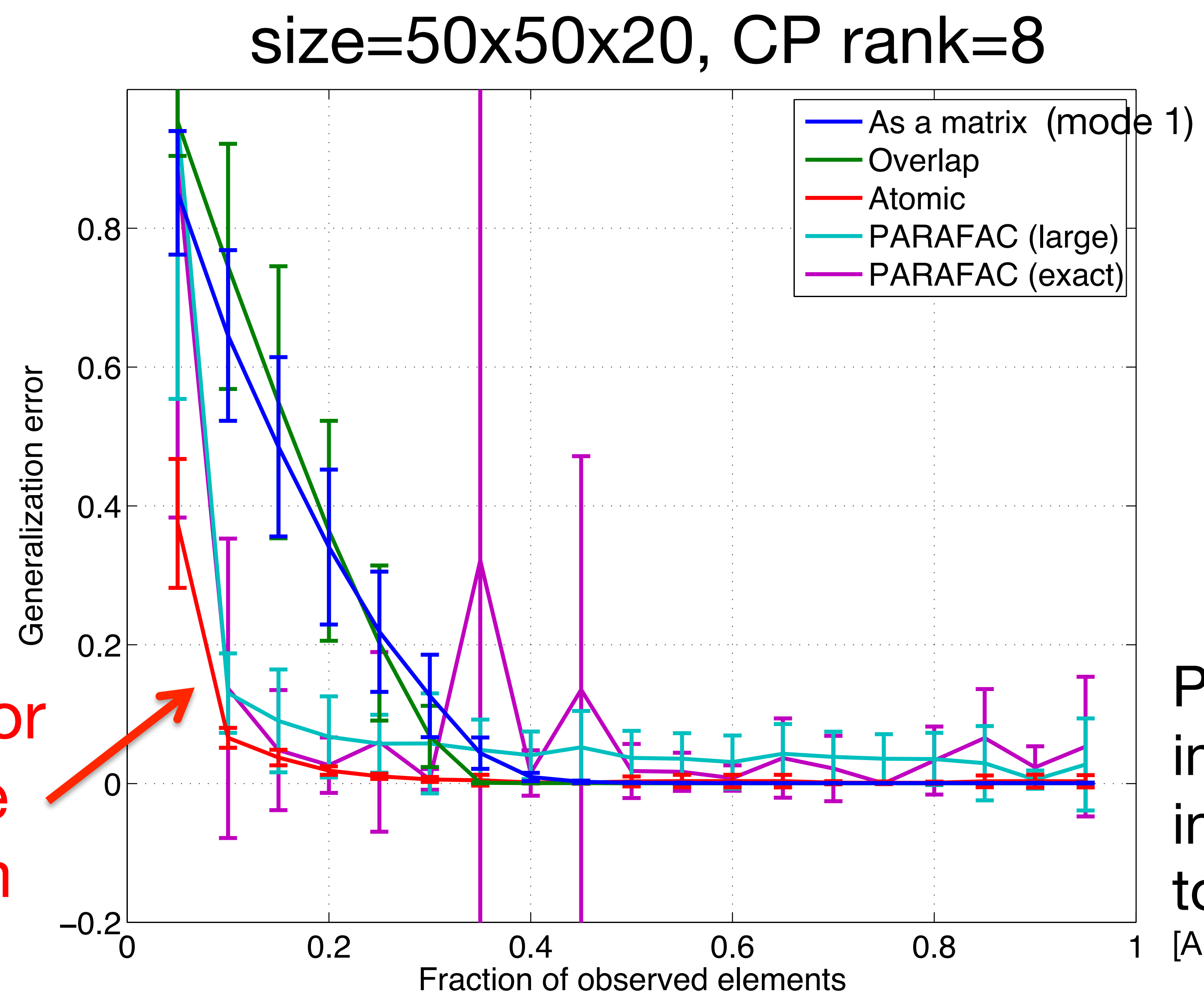
Tensor operator norm

Greedy algorithm for $\mathrm{prox}_\lambda(W)$

1. Let R=W.
2. Compute $\|R\|_{op}$
   if $\|R\|_{op} \leq \lambda$, done. Return W-R
   otherwise, $R=R+(\lambda-\|R\|_{op})\, u \cdot v \cdot w$
3. Go to 2.

Tensor completion experiment

(λ→0)

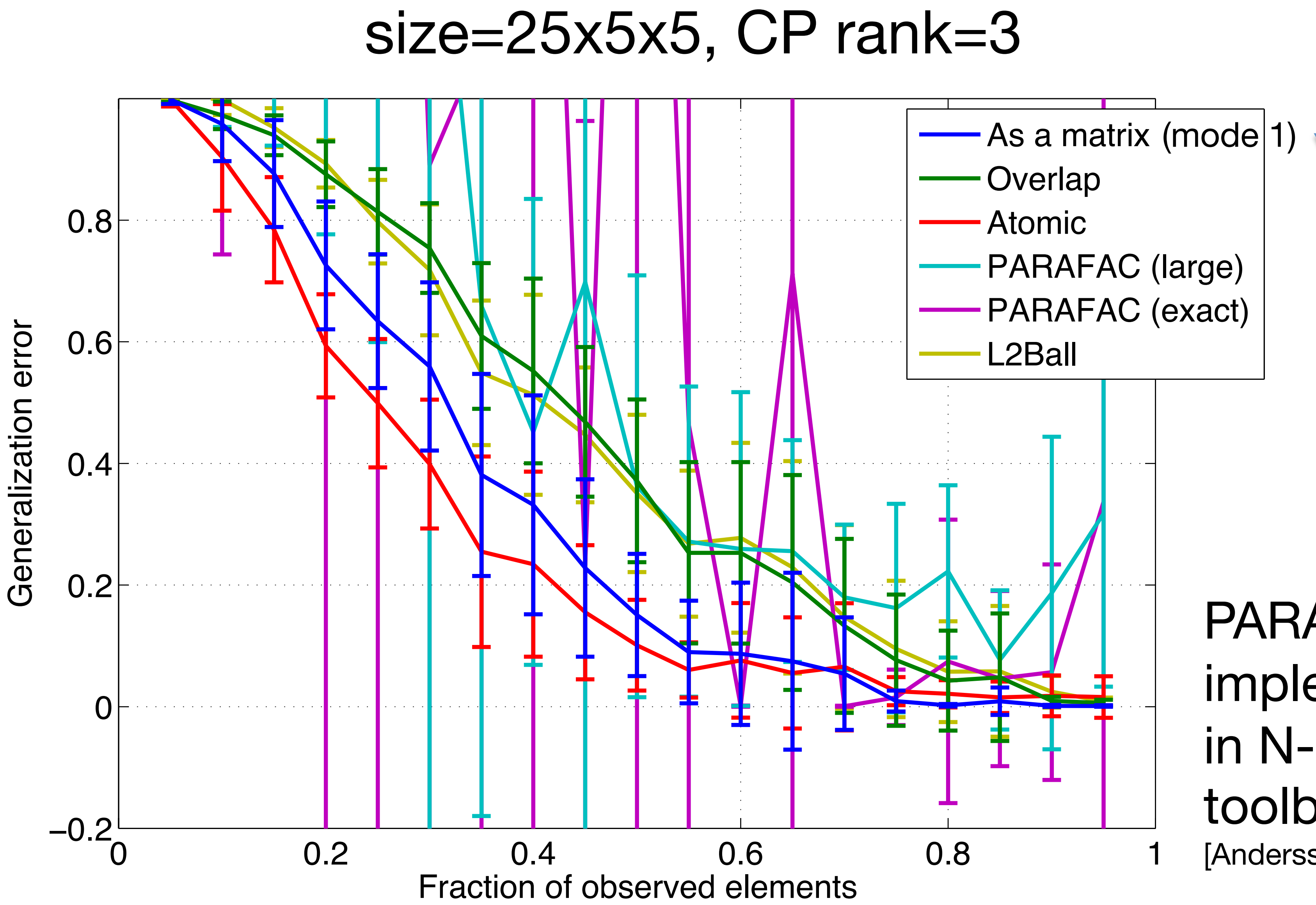


tensor trace norm

PARAFAC implemented in N-way toolbox [Andersson & Bro 00]

Balanced vs. unbalanced

(λ→0)



balanced 25x25

PARAFAC implemented in N-way toolbox

[Andersson & Bro 00]

Summary

- Tensor decomposition via convex optimization
  - Fast and stable algorithm for tensor decomposition
  - Rank selection is replaced by regularization parameter selection
- Limitation of the overlapped trace norm
  - unbalancedness of the unfolding
  - balanced unfolding
- Optimization statistics trade-off
  - balanced trace norm requires less samples but more computation
  - tensor trace norm requires only O(n) samples but seems intractable

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Thank you!