



Practical Leverage-Based Sampling for Low-Rank Tensor Decomposition

Tamara G. Kolda

Sandia National Labs, Livermore, CA www.kolda.net

Joint work with Brett Larsen Stanford University

Supported by the DOE Office of Science Advanced Scientific Computing Research (ASCR) Applied Mathematics. Sandia National Laboratories is a multimission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC., a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA-0003525.

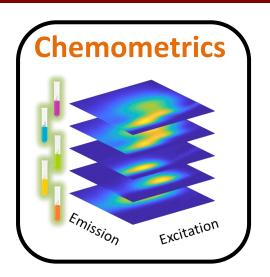


llustration by Chris Brigmar

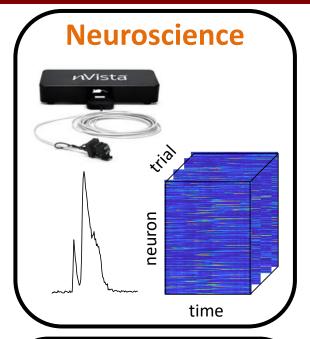


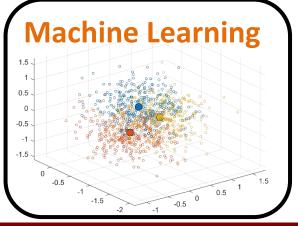


- Chemometrics: Emission x Excitation x Samples (Fluorescence Spectroscopy)
- Neuroscience: Neuron x Time x Trial
- Criminology: Day x Hour x Location x Crime (Chicago Crime Reports)
- Machine Learning: Multivariate Gaussian Mixture Models Higher-Order Moments
- Transportation: Pickup x Dropoff x Time (Taxis)
- Sports: Player x Statistic x Season (Basketball)
- Cyber-Traffic: IP x IP x Port x Time
- Social Network: Person x Person x Time x Interaction-Type
- Signal Processing: Sensor x Frequency x Time
- Trending Co-occurrence: Term A x Term B x Time













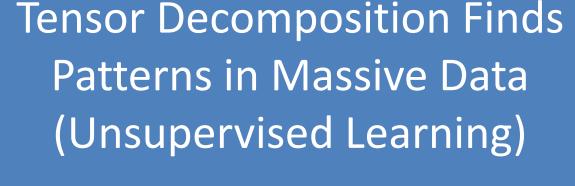


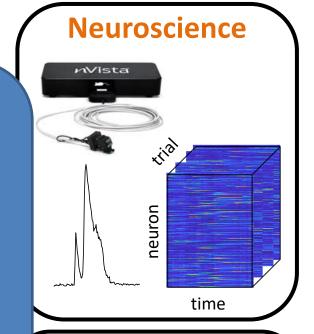
Tensors Come From Many Applications

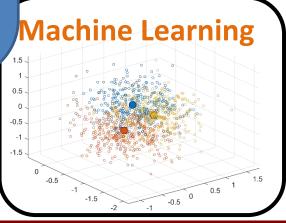
 Chemometrics: Emission x Excitation x Samples (Fluorescence Spectroscopy)

Chemometrics

- Neuroscience:
- Criminology: D
 (Chicago Crime
- Machine Learr Mixture Mode
- Transportation
- Sports: Player
- Cyber-Traffic:
- Social Network
 Interaction-Type
- Signal Processing: Sensor x Frequency x Time
- Trending Co-occurrence: Term A x Term B x Time

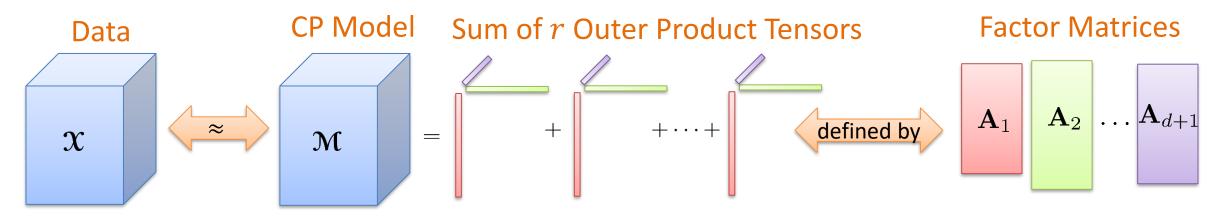








Tensor Decomposition Identifies Factors



$$\mathbf{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_{d+1}}$$

$$x_i = x(i_1, i_2, \dots, i_{d+1})$$

$$\mathbf{M} = [\![\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_{d+1}]\!] \in \mathbb{R}^{n_1 \times n_2 \times \dots \times n_{d+1}}$$

$$x_i = x(i_1, i_2, \dots, i_{d+1})$$
 $m_i = m(i_1, i_2, \dots, i_{d+1}) = \sum_{j=1}^r \prod_{k=1}^{d+1} a_k(i_k, j)$

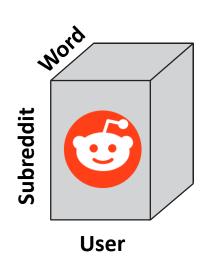
$$\mathbf{A}_k \in \mathbb{R}^{n_k imes r}$$
Model Rank





Example Sparse Multiway Data: Reddit

- Reddit is an American social news aggregator, web content rating, and discussion website
 - A "subreddit" is a discussion forum on a particular topic
- Tensor obtained from frost.io (http://frostt.io/tensors/reddit-2015/)
 - Built from reddit comments posted in the year 2015
 - Users and words with less than 5 entries have been removed



Reddit Tensor

8 million users

200 thousand subreddits

8 million words

4.7 billion non-zeros $(10^{-8}\%)$

106 gigabytes

 $x(i, j, k) = \log (1 + \text{the number of times user } i \text{ used word } j \text{ in subreddit } k)$

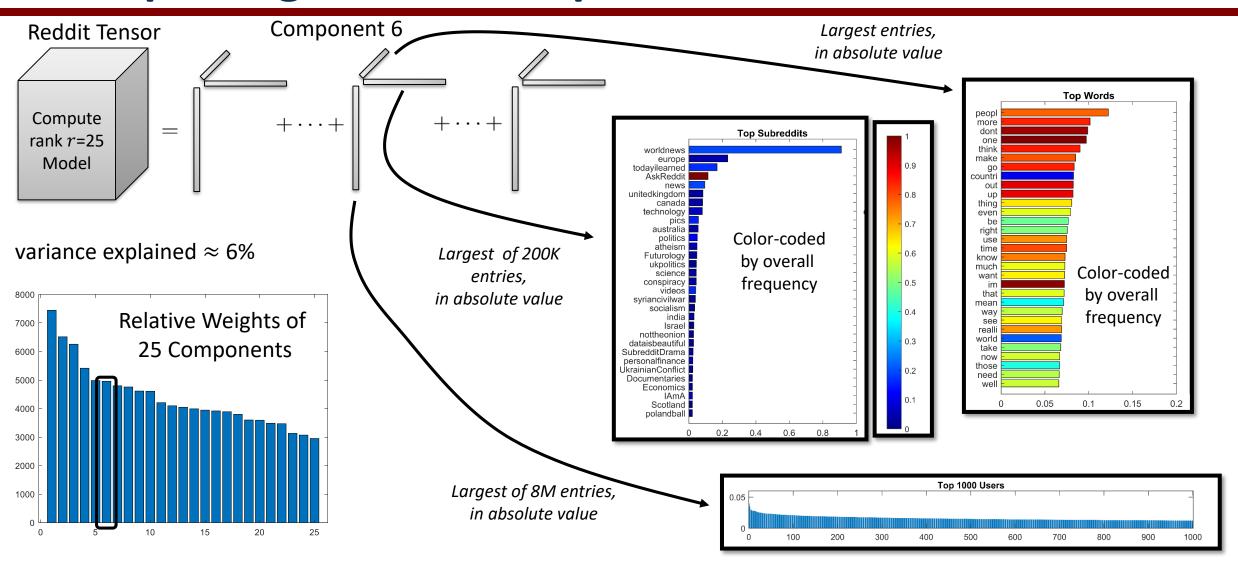
Used a rank r = 25 decompsition

Smith et al (2017). "FROSTT: The Formidable Open Repository of Sparse Tensors and Tools"





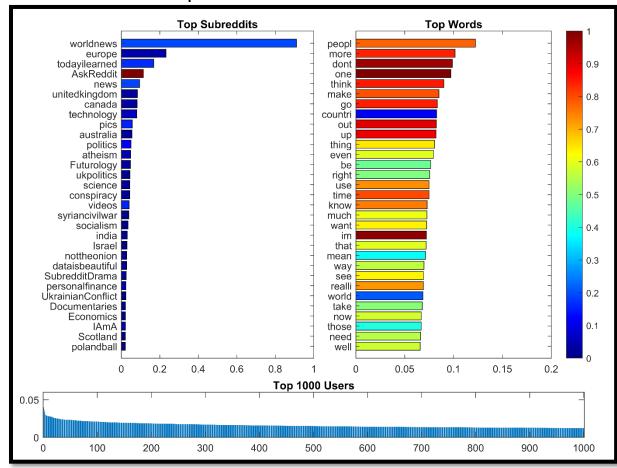
Interpreting Reddit Components



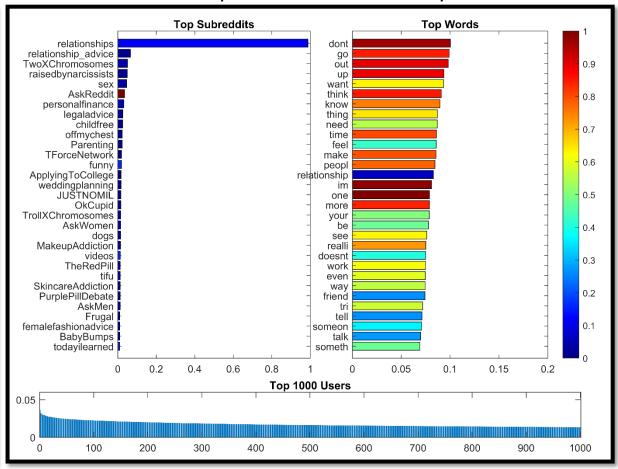




Component #6: International News



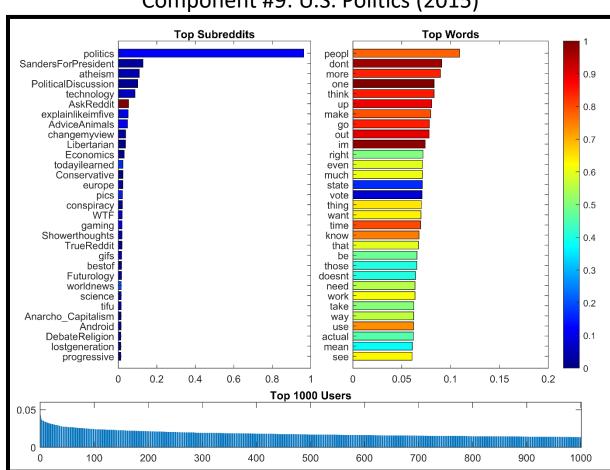
Component #8: Relationships



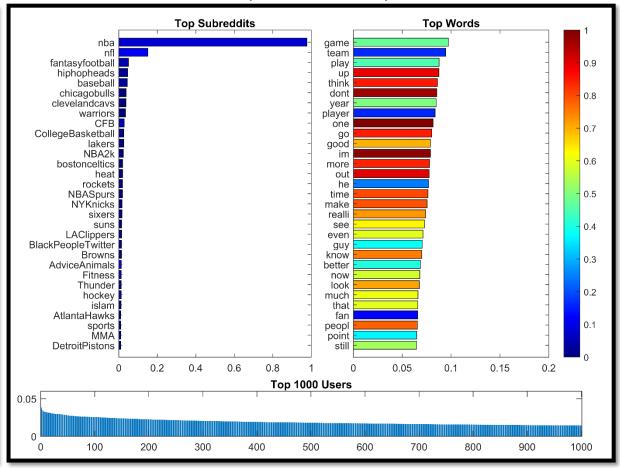




Component #9: U.S. Politics (2015)



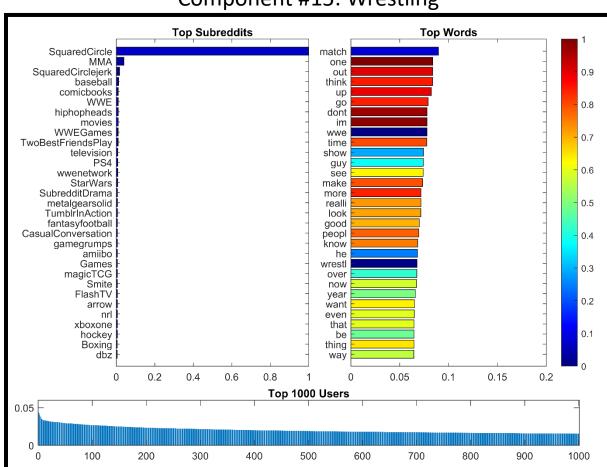
Component #11: Sports



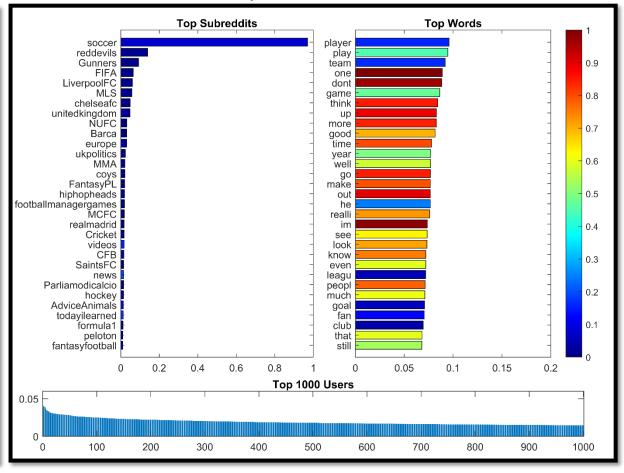




Component #15: Wrestling



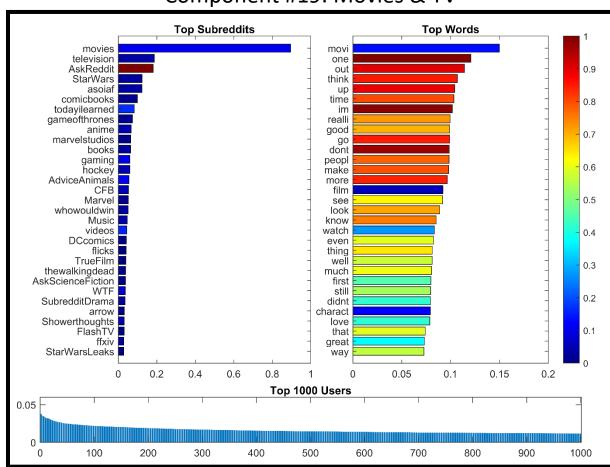
Component #18: Soccer



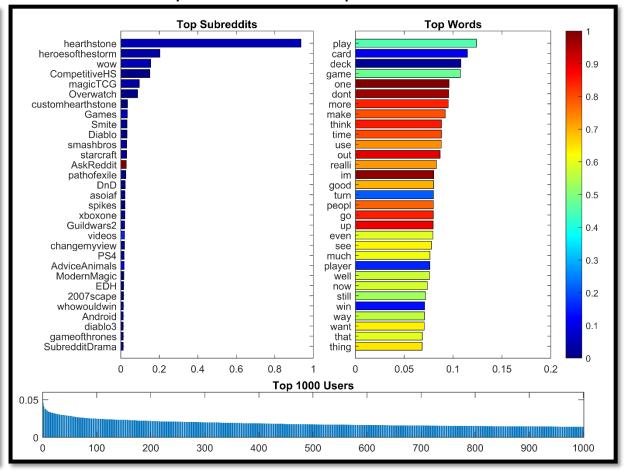




Component #19: Movies & TV



Component #18: Computer Card Game



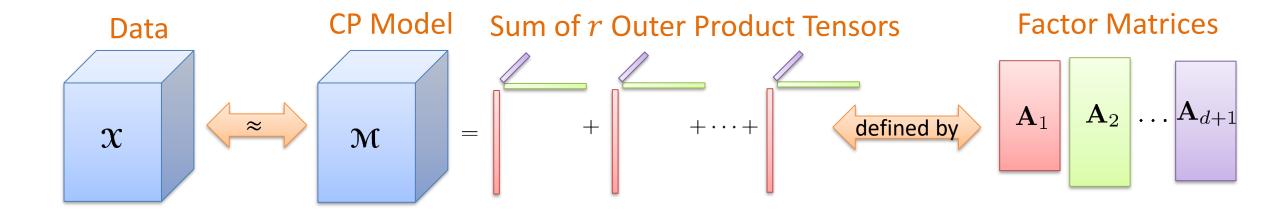


Model Rank

Tensor Decomposition Identifies Factors

 $x_i = x(i_1, i_2, \dots, i_{d+1})$ $m_i = m(i_1, i_2, \dots, i_{d+1}) = \sum_{i=1}^{r} \prod_{j=1}^{d+1} a_k(i_k, j)$

 $\mathbf{X} \in \mathbb{R}^{n_1 \times n_2 \times \cdots \times n_{d+1}}$



 $\mathbf{M} = [\![\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_{d+1}]\!] \in \mathbb{R}^{n_1 \times n_2 \times \dots \times n_{d+1}}$

 $i = 1 \ k = 1$

<u>Key Idea</u>: Alternate among the d factor matrices, fixing all but that one and solving. Each subproblem is linear least squares.

Prototypical CP Least Squares Problem has



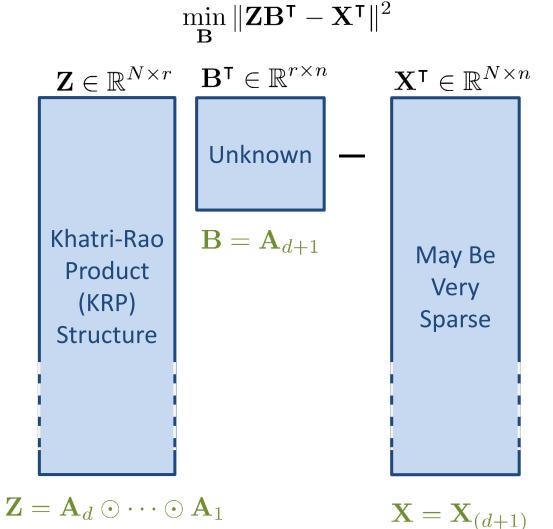


$$N \gg r, n$$

Linking back to mode-(d+1)least squares subproblem

$$N = \prod_{k=1}^{d} n_k$$

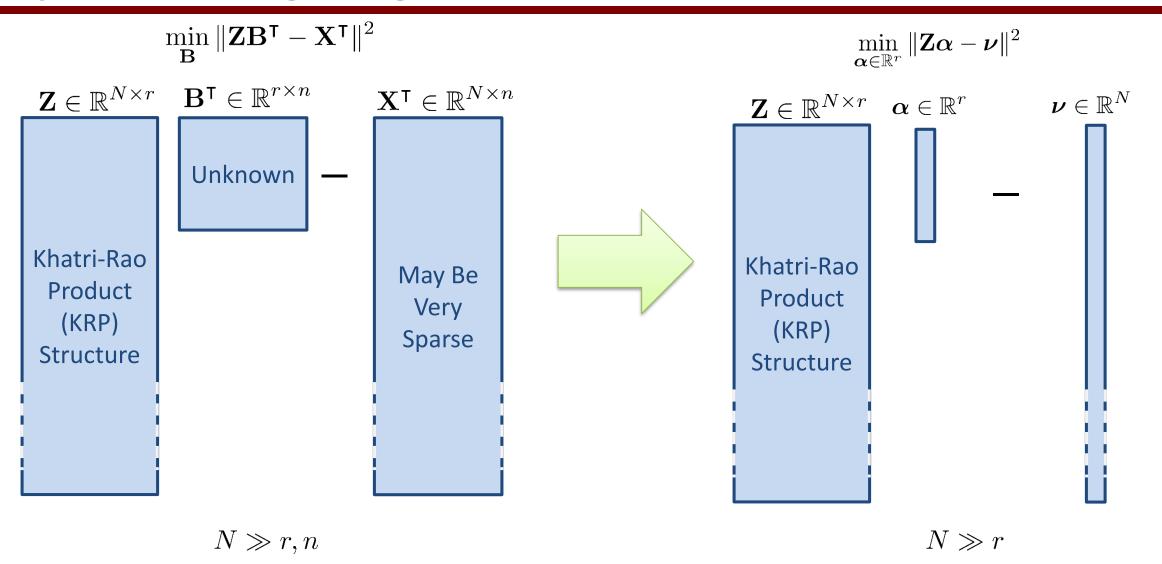
$$n = n_{d+1}$$



- KRP costs O(Nr) to form
- System costs $O(Nnr^2)$ to solve
- KRP structure
 - Cost reduced to O(Nnr)
- KRP structure + data sparse
 - Cost reduced to $O(r \operatorname{nnz}(\mathbf{X}))$

For Ease of Discussion: Simplify KRP Least Squares to Single Right-Hand Side



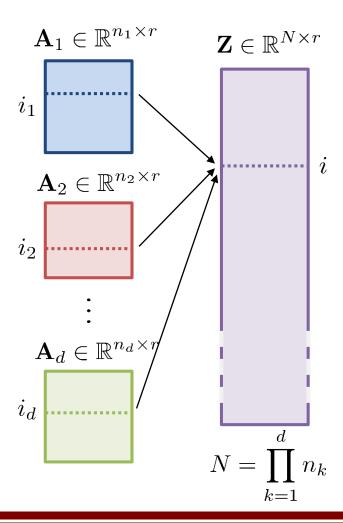


Structure of Khatri-Rao Product (KRP): Hadamard Combinations of Rows of Inputs



KRP of d Matrices: $\mathbf{Z} = \mathbf{A}_d \odot \cdots \odot \mathbf{A}_1$

Number of columns is the same in all input matrices, but number of rows varies



Each row of KRP is Hadamard product of specific rows in Factor Matrices:

$$\mathbf{Z}(i,:) = \mathbf{A}_1(i_1,:) * \cdots * \mathbf{A}_d(i_d,:)$$

where

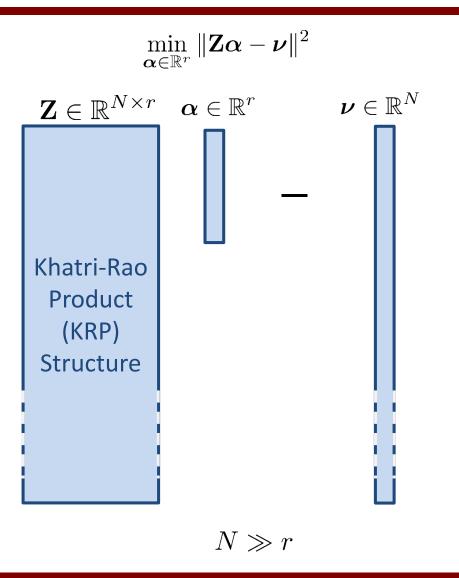
$$i = (n_{d-1} \cdots n_1)(i_d - 1) + (n_{d-2} \cdots n_1)(i_{d-1} - 1) + \cdots + n_1(i_2 - 1) + i_1 \in [N]$$

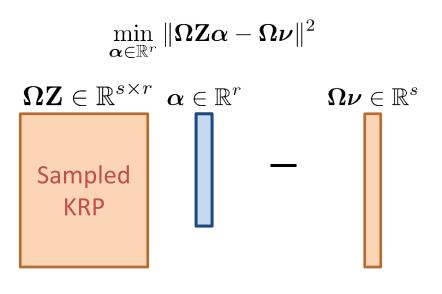
1-1 Correspondence between *linear index and multi index:*

$$i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \dots \otimes [n_d]$$

Ingredient #1: Sample Subset of Rows in Overdetermined Least Squares System







Complexity reduced from O(Nr) to $O(sr^2)$

Key surveys:

M. W. Mahoney, *Randomized Algorithms for Matrices and Data*, 2011; D. P. Woodruff, *Sketching as a Tool for Numerical Linear Algebra*, 2014

How sample so that solution of sampled problem yields something close to the optimal residual of the original problem?

Ingredient #2: Weight Sampled Rows by Probability of Selection to Eliminate Bias



Probability distribution on rows of linear system

$$\left(\sum_{i=1}^{N} p_i = 1\right)$$

Not specifying yet how these probabilities are selected

Pick a single random index ξ with probability p_{ξ}

Choose

$$\mathbf{\Omega} = \begin{bmatrix} 0 & \cdots & 0 & \frac{1}{\sqrt{p_{\xi}}} & 0 & \cdots & 0 \end{bmatrix} \in \mathbb{R}^{N \times 1}$$
 ξ th entry

Then (assuming all p_i positive) the sampled the sampled residual equals true residual in expectation:

$$\mathbb{E}\|\mathbf{\Omega}\mathbf{Z}\boldsymbol{\alpha} - \mathbf{\Omega}\boldsymbol{\nu}\|^2 = \sum_{i=1}^{N} p_i \left(\left\| \frac{1}{\sqrt{p_i}} \mathbf{Z}(i,:)\boldsymbol{\alpha} - \frac{1}{\sqrt{p_i}} \nu_i \right\|^2 \right)$$
$$= \|\mathbf{Z}\boldsymbol{\alpha} - \boldsymbol{\nu}\|^2$$

Pick a s random indices ξ_j (with replacement) such that $P(\xi_j = i) = p_i$.

Choose $\mathbf{\Omega} \in \mathbb{R}^{s imes N}$ such that

Not specifying yet how s is determined

$$\omega(j,i) = \begin{cases} \frac{1}{\sqrt{sp_i}} & \text{if } \xi_j = i\\ 0 & \text{otherwise} \end{cases}$$

Each row has a single nonzero!

Then, as before, we have:

$$\|\mathbb{E}\|\Omega \mathbf{Z} lpha - \Omega
u\|^2 = \|\mathbf{Z} lpha -
u\|^2$$

Survey: D. P. Woodruff, Sketching as a Tool for Numerical Linear Algebra, 2014

Theory Review: Connecting Probabilities, Leverage Scores, and Number of Samples



 $\|\mathbf{Z}\boldsymbol{\alpha} - \boldsymbol{\nu}\|^2 \text{ with } \mathbf{Z} \in \mathbb{R}^{N \times r}, \, \boldsymbol{\nu} \in \mathbb{R}^N$ Given linear system:

> Pick a s random indices ξ_i such that And random

 $P(\xi_i = i) = p_i$ and define sampling matrix:

$$\mathbf{\Omega} \in \mathbb{R}^{s \times N} \text{ with } \omega(j, i) = \begin{cases} \frac{1}{\sqrt{sp_i}} & \text{if } \xi_j = i\\ 0 & \text{otherwise} \end{cases}$$

Solve sampled

problem:

$$ilde{oldsymbol{lpha}}_* \equiv rg\min_{oldsymbol{lpha} \in \mathbb{R}^r} \| oldsymbol{\Omega} \mathbf{Z} oldsymbol{lpha} - oldsymbol{\Omega} oldsymbol{
u} \|_2^2$$

Get probabilistic

error bound:

For error $\epsilon \in (0,1)$, confidence

 $1 - \delta \in (0,1)$, we have

$$P(\|\mathbf{Z}\tilde{\alpha}_* - \boldsymbol{\nu}\|_2^2 \le (1 + O(\epsilon))\|\mathbf{Z}\alpha_* - \boldsymbol{\nu}\|_2^2) > 1 - \delta$$

when number of samples satisfies:

$$s = O(\epsilon^{-2} \ln \left(\frac{r}{\delta}\right) r \beta^{-1})$$

where β -term:

$$\beta = \min_{i \in [N]} \frac{r \, p_i}{\ell_i(\mathbf{Z})} \in (0,1]$$
Leverage score

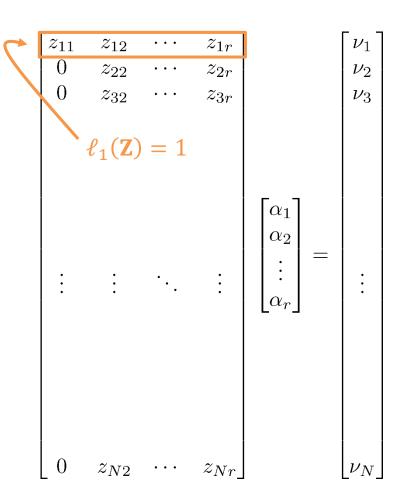
Want β as big as possible! Ideally, $p_i = \ell_i(\mathbf{Z})/r$ for all $i \in [N]$, but ...

A. Eshragh, et al., LSAR: Efficient Leverage Score Sampling Algorithm for the Analysis of Big Time Series Data, arXiv:1911.12321, 2019; D. P. Woodruff, Sketching as a Tool for Numerical Linear Algebra, 2014

Ingredient #3: Leverage Scores Key to Limiting Samples (but too Expensive to Compute)







$$\mathbf{Z} \in \mathbb{R}^{N imes r}$$

Leverage score:

Let **Q** be any orthonormal basis of the column space of **Z**.

Leverage score of row *i*:

$$\ell_i(\mathbf{Z}) = \|\mathbf{Q}(i,:)\|_2^2 \in [0,1]$$

Coherence:

$$\mu(\mathbf{Z}) = \max_{i \in [N]} \ell_i(\mathbf{Z})$$
$$r/N \le \mu(\mathbf{Z}) \le 1$$

Rough Intuition:

Key rows have high leverage score

What if we do uniform sampling? $p_i = \frac{1}{N}$ for all $i \in [N]$,

$$\beta = \min_{i \in [N]} \frac{r \, p_i}{\ell_i(\mathbf{Z})} = \min_{i \in [N]} \frac{r/N}{\ell_i(\mathbf{Z})}$$
$$s = O(\epsilon^{-2} \ln(r) \, r \beta^{-1})$$

Case 1: $\mu(\mathbf{Z}) = r/N$ (incoherent)

$$\Rightarrow \beta = 1 \Rightarrow s = O(\epsilon^{-2} \ln(r) r)$$

Case 2: $\mu(\mathbf{Z}) = 1$ (coherent)

$$\Rightarrow \beta = r/N \Rightarrow s = O(\epsilon^{-2} \ln(r) N)$$

In Case 2, prefer $p_i = \ell_i(\mathbf{Z})/r$, but costs $O(Nr^2)$ to compute leverage scores!

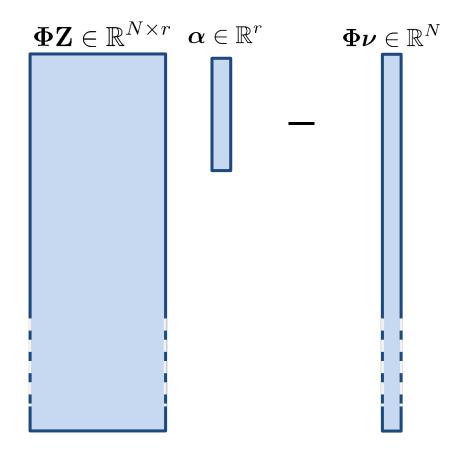
Survey: D. P. Woodruff, Sketching as a Tool for Numerical Linear Algebra, 2014

Aside: Uniform Sampling Okay for "Mixed" Dense Tensors (Inapplicable to Sparse)







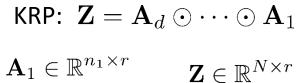


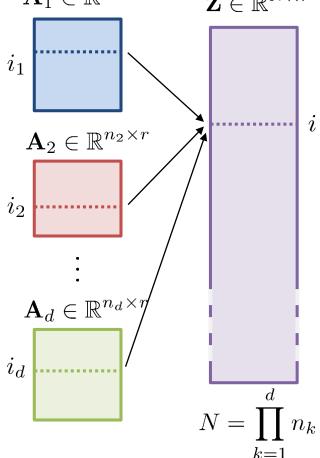
- Choose Φ so that all leverage scores of ΦZ approximately equal, then uniform sampling yields $\beta \approx 1$
 - "Uniformize" the leverage scores per Mahoney
 - Fast Johnson-Lindenstrauss Transform (FJLT) uses random rows of matrix transformed by FFT and Rademacher diagonal
 - FJLT cost per iteration: $O(rN \log N)$
- Gaining Efficiency for KRP matrices
 - Transform individual factor matrices before forming Z
 - Sample rows of Z implicitly
 - Kronecker Fast Johnson-Lindenstrauss Transform (KFJLT)
 - Special handling of right-hand side with preprocessing costs
 - KFJLT cost per iteration: $O(r\sum_k n_k \log n_k + sr^2)$
- References
 - C. Battaglino, G. Ballard, T. G. Kolda. A Practical Randomized CP Tensor Decomposition. SIAM Journal on Matrix Analysis and Applications, Vol. 39, No. 2, pp. 876-901, 26 pages, 2018. https://doi.org/10.1137/17M1112303
 - R. Jin, T. G. Kolda, R. Ward. Faster Johnson-Lindenstrauss Transforms via Kronecker Products, 2019. http://arxiv.org/abs/1909.04801

Ingredient #4: Exploit KRP Structure to Bound Leverage Scores









Upper Bound on Leverage Score

Lemma (Cheng et al., NIPS 2016;

Battaglino et al., SIMAX 2018):

$$\ell_i(\mathbf{Z}) \le \prod_{k=1}^{a} \ell_{i_k}(\mathbf{A}_k)$$

Too expensive to calculate $O(Nr^2)$

Cheap to calculate individual leverage scores $O(r^2 \sum_k n_k)$

Set probability of sampling row i to:

$$p_i \equiv \frac{1}{r^d} \prod_{k=1}^d \ell_{i_k}(\mathbf{A}_k)$$

Tensor Least Squares Sketching with Leverage Scores

Thm: Using this sampling probability yields $(1+\epsilon)$ accuracy w.h.p. with number of rows

$$s = O(r^d \log(r/\delta)/\epsilon^2)$$

1-1 Correspondence between *linear index and multi index:*

$$i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \dots \otimes [n_d]$$

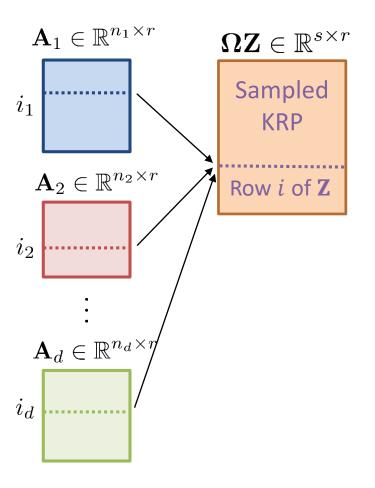
N possible combinations corresponding to all rows of **Z**!

Ingredient #5: Randomly Sample Rows of KRP Using Implicit Leverage Score Bounds









Probability of sampling row i:

$$p_i \equiv \frac{1}{r^d} \prod_{k=1}^d \ell_{i_k}(\mathbf{A}_k)$$

- Recall our goal: Pick s random indices ξ_i such that $Pig(\xi_i=iig)=p_i$
- For j-th sample for j = 1, ..., s:
 - Sample one row from each factor matrix such that $\operatorname{Prob}(\operatorname{row} i_k) = \ell_{i_k}(\mathbf{A}_k)/r$
 - Set $\xi_i = i$, where $P(\xi_i = i) = p_i$
 - Compute Hadamard products of corresponding rows of factor matrices
 - Weight by $1/\sqrt{sp_i}$
- Never computes...
 - Matrix **Z** nor its leverage scores
 - Weight matrix Ω
- Computing factor matrix leverage scores costs only $O(r^2 \sum_k n_k)$
 - Versus $O(Nr^2)$ for computing leverage scores from **Z**

1-1 Correspondence between linear index and multi index:

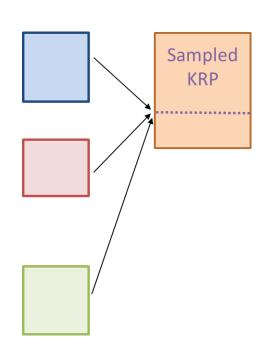
$$i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \dots \otimes [n_d]$$





Ingredient #6: Combine Repeated Rows

<u>Problem</u>: Concentrated sampling probabilities identify a few key rows but can lead to many repeats!



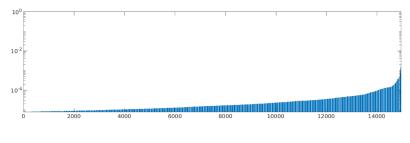
Least Squares Problems from Real-world Tensor Data Sets

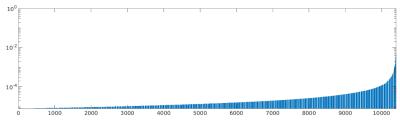
Example 1:
$$N = 3.2e12$$
, $s = 2^{17}$, $\tau = \frac{1}{s} = 8e-6$ $\mathcal{D} = \{i : p_i > \tau\}$, $|\mathcal{D}| \approx 15000$, $\sum_{i \in \mathcal{D}} p_i = 0.51$

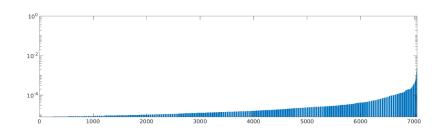
Example 2:
$$N = 8.7e12$$
, $s = 2^{17}$, $\tau = \frac{1}{s} = 8e-6$
 $\mathcal{D} = \{i : p_i > \tau\}$, $|\mathcal{D}| \approx 10000$, $\sum_{i \in \mathcal{D}} p_i = 0.41$

Example 3:
$$N=8.6 \mathrm{e} 12$$
, $s=2^{17}$, $\tau=\frac{1}{s}=8 \mathrm{e} -6$ $\mathcal{D}=\{i:p_i>\tau\}, |\mathcal{D}|\approx 7000, \sum_{i\in\mathcal{D}}p_i=0.25$

Combining repeat rows \Rightarrow 2-20X speedup

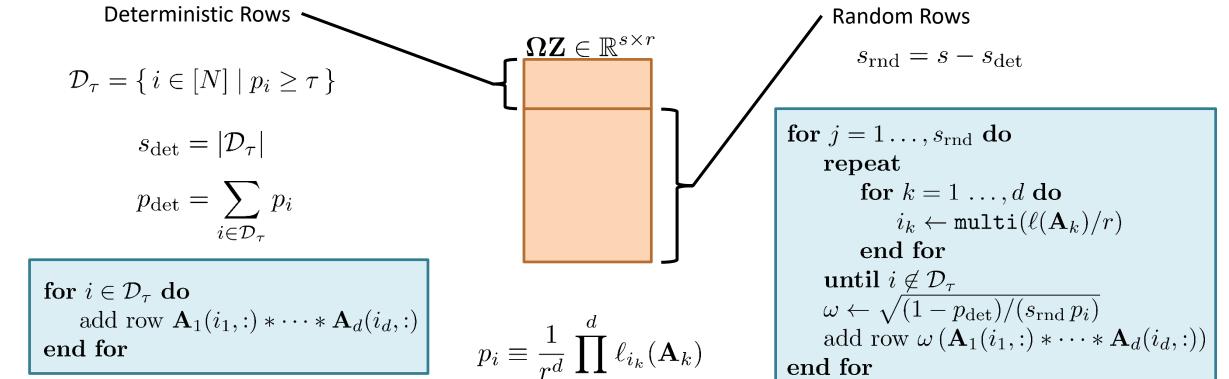






Ingredient #7: Hybrid Deterministic and **Randomly-Sampled Rows**





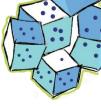
end for

1-1 Correspondence between linear index and multi index:

$$i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \dots \otimes [n_d]$$

Ingredient #9: Find All High-Probability Rows without Computing All Probabilities





Recall

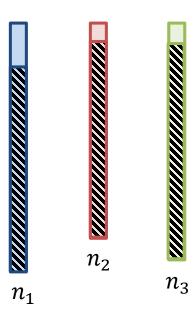
$$p_i \equiv \frac{1}{r^d} \prod_{k=1}^d \ell_{i_k}(\mathbf{A}_k)$$

• For given tolerance $\tau > 1/N$, define the set of deterministic rows to include

$$\mathcal{D}_{\tau} = \{ i \in [N] \mid p_i \ge \tau \}$$

- Compute without computing all p_i values
- A few high leverage scores means all the others are necessarily low!
- Use bounding procedure to eliminate most options
- Compute products of at most a top few leverage scores in each mode

Sorted Leverages Scores (Descending)

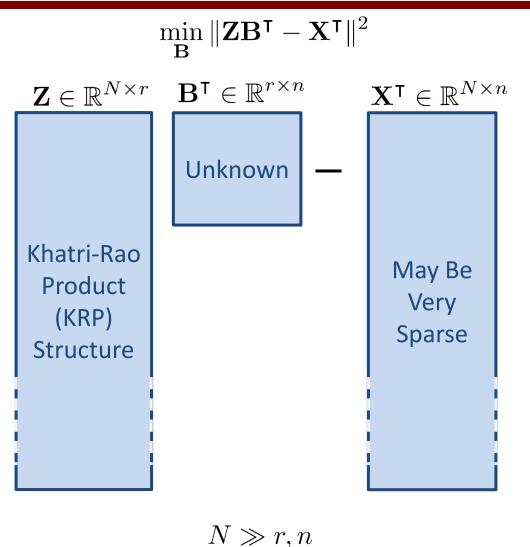


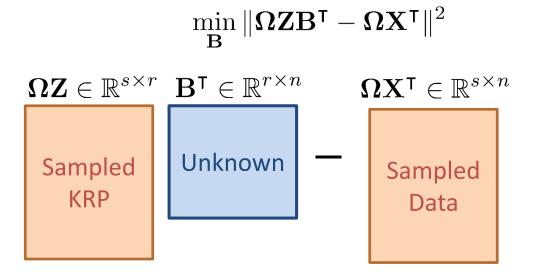
1-1 Correspondence between linear index and multi index:

$$i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \dots \otimes [n_d]$$

Remember the Original Problem – Need to Sample the Right-Hand Side as Well



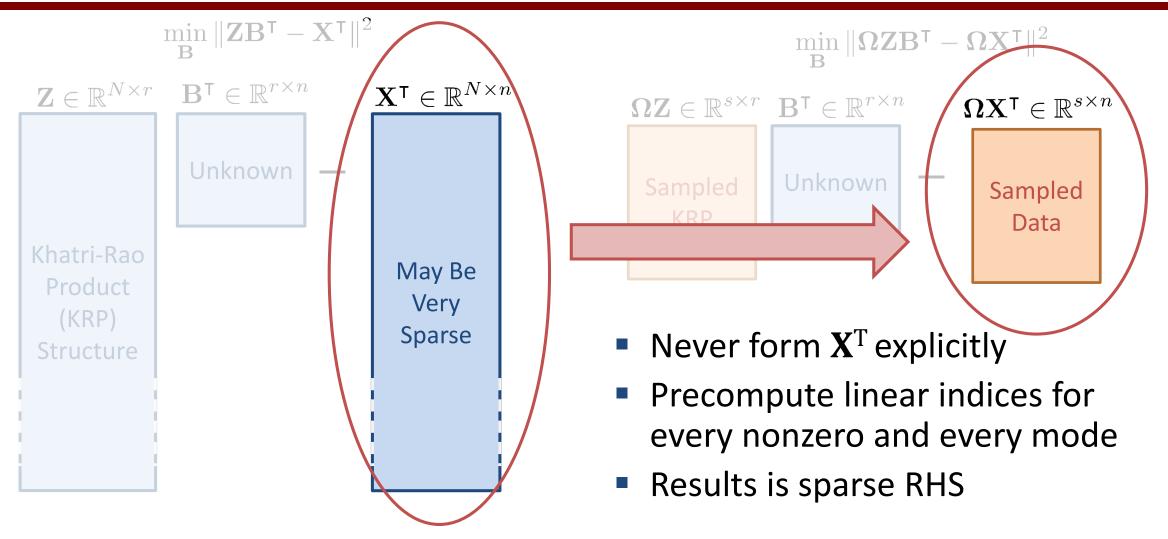




Complexity reduced from O(Nrn) to $O(sr^2n)$

Ingredient #9: Efficiently Extract RHS from (Sparse) Unfolded Data Tensor





Similar in spirit to ideas for dense tensors in Battaglino et al., SIMAX 2018

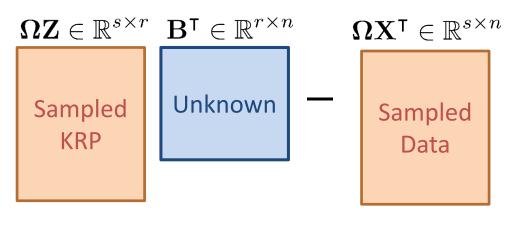


Numerical Results

Solution Quality as Number of Samples Increase and Hybrid Improvements

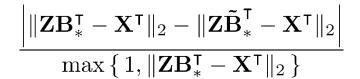


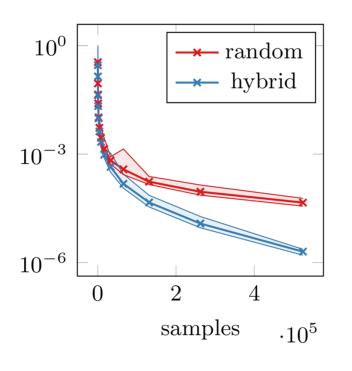
Single Least Squares Problem with N = 46M rows, r = 10 columns, n = 183 right-hand sides



$$\tilde{\mathbf{B}}_* \equiv \arg\min_{\mathbf{B} \in \mathbb{R}^r} \|\mathbf{\Omega} \mathbf{Z} \mathbf{B}^\intercal - \mathbf{\Omega} \mathbf{X}^\intercal\|_2^2$$

$$\mathbf{B}_* \equiv \arg\min_{\mathbf{B} \in \mathbb{R}^r} \|\mathbf{Z}\mathbf{B}^\intercal - \mathbf{X}^\intercal\|_2^2$$

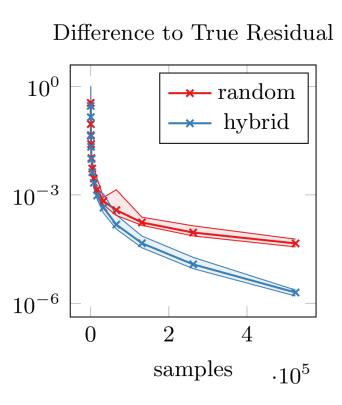


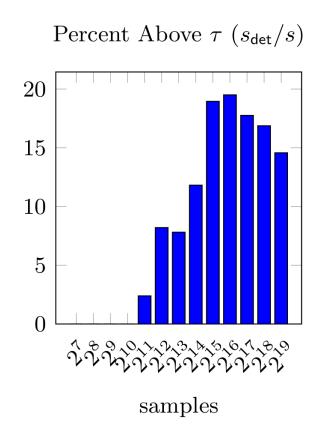


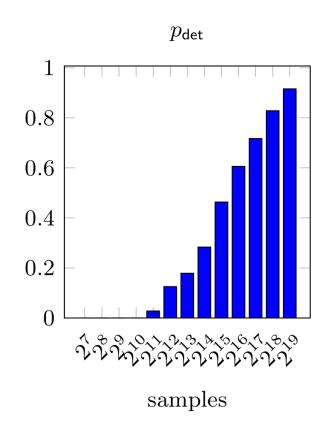
Deterministic Can Account for Substantial Portion of Probability



Single Least Squares Problem with N = 46M rows, r = 10 columns, n = 183 right-hand sides

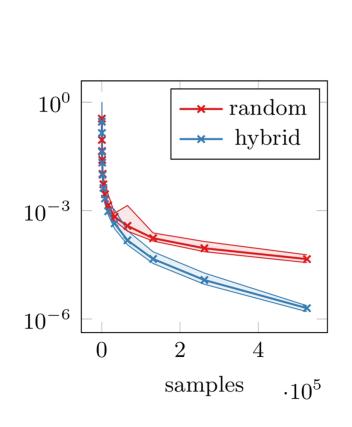


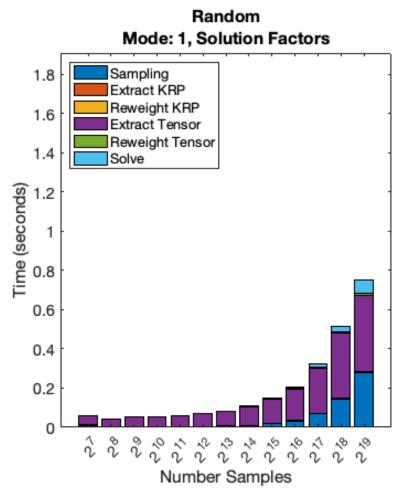


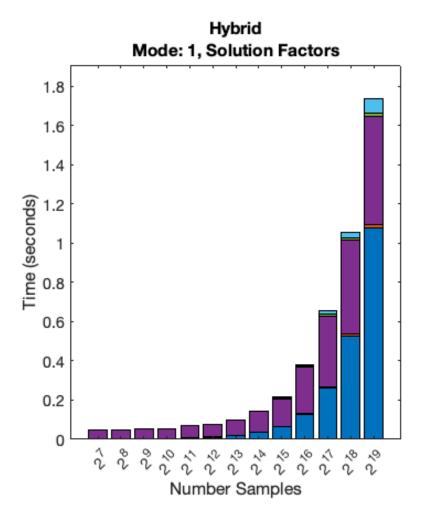


Some Trade-off Between Accuracy and Expense for Deterministic



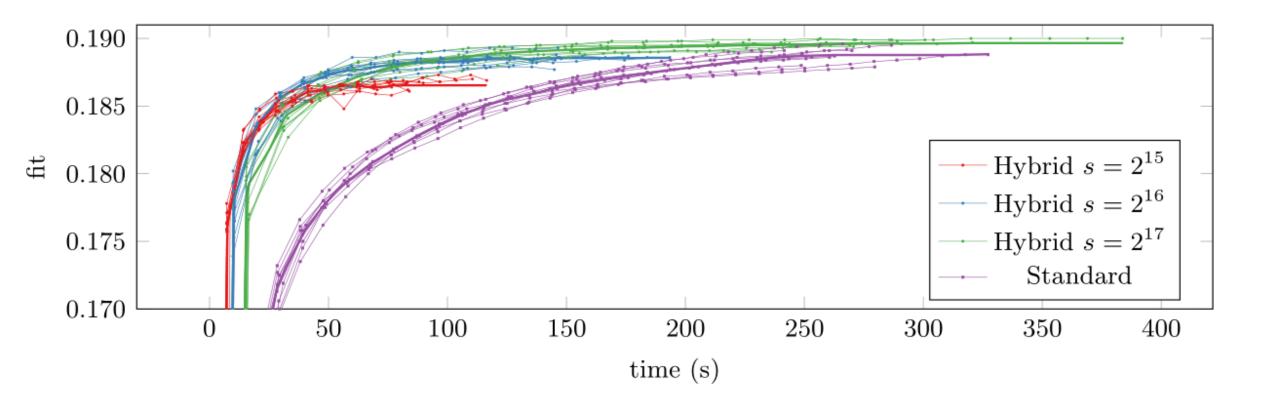






CP-ARLS-LEV (Hybrid) Comparable to CP-ALS (Standard) on Small Uber Problem

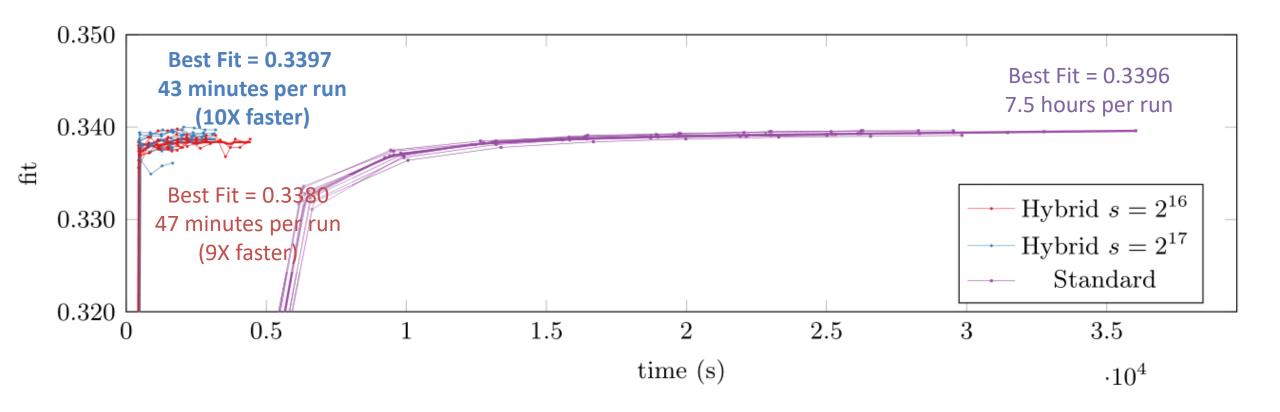




Uber Tensor: 183 x 24 x 1140 x 1717 Uber Tensor with 3M nonzeros (0.038% dense). Rank r = 25 CP decomposition

Over 9X Speed-up for Amazon Tensor with 1.7 Billion Nonzeros

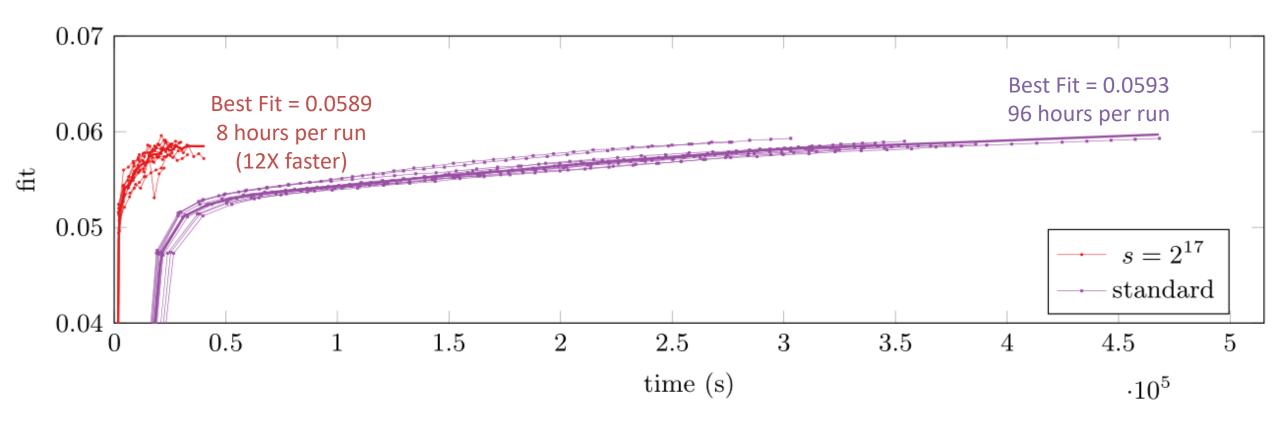




Amazon Tensor: $4.8M \times 1.8M \times 1.8M$ Amazon Tensor with 1.7B nonzeros. Rank r = 25 CP decomposition

Over 12X Speed-up for Reddit Tensor with 4.6 Billion Nonzeros (106 GB)





Amazon Tensor: 8.2M x 0.2M x 8.1M Reddit Tensor with 4.7B nonzeros. Rank r = 25 CP decomposition





Conclusions & Future Work

- How to make CP tensor decomposition faster for largescale sparse tensors? Matrix sketching
- How to avoid repeated samples? Combine repeat rows or deterministically include high-probability rows
- How to efficiently sample? Sample independently from each factor matrix to build KRP
- How to extract data for RHS from data tensor? Precompute linear indices for tensor fibers
- Overall result: Order-of-magnitude speed-ups
- Many open problems: How to pick # samples (per mode even), deterministic threshold, robust stopping conditions, sampling based on data as well as KRP, parallelization of method, etc.

Contact Info: Brett <u>bwlarsen@stanford.edu</u>, Tammy <u>tgkolda@sandia.gov</u>

