

Practical Leverage-Based Sampling for Low-Rank Tensor Decomposition

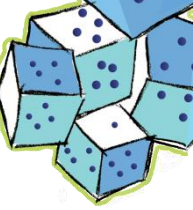
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Joint work with
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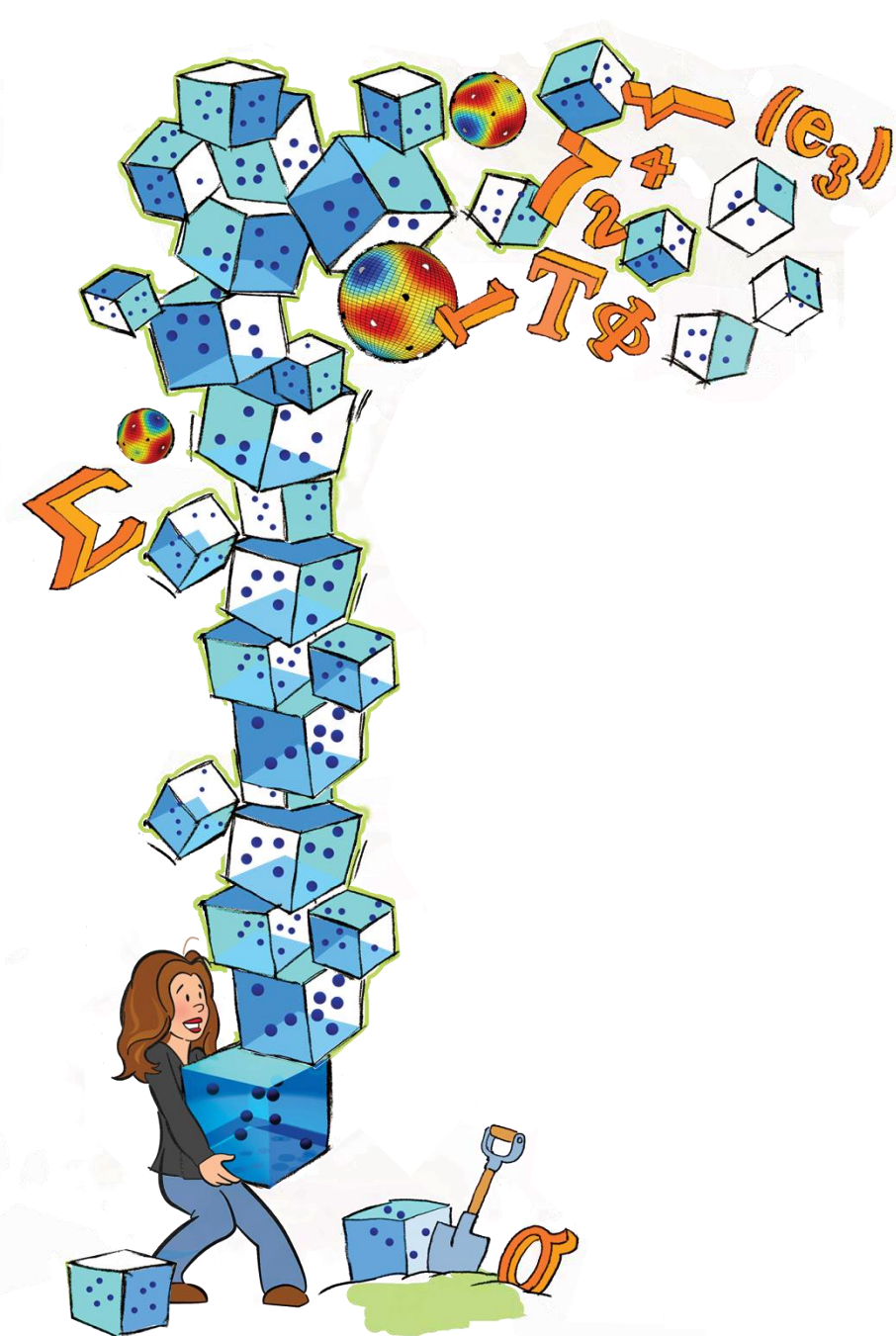
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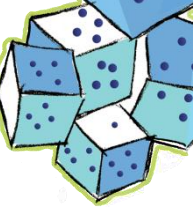




Funding

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- Brett was also funded by DOE Computational Science Graduate Fellowship (CSGF), administered by the Krell Institute

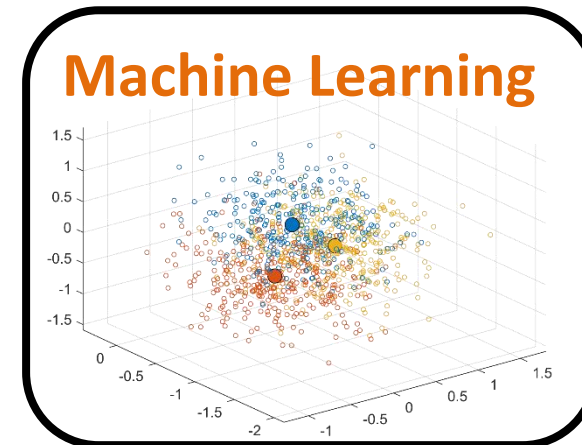
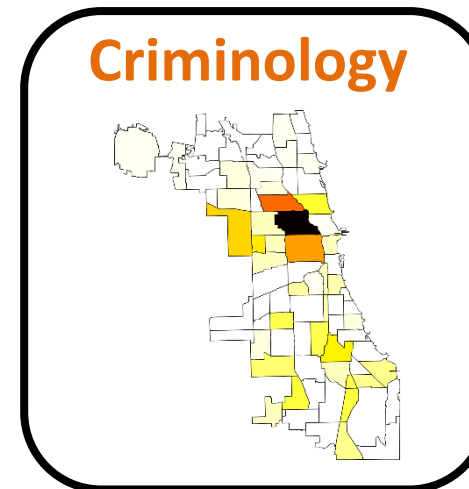
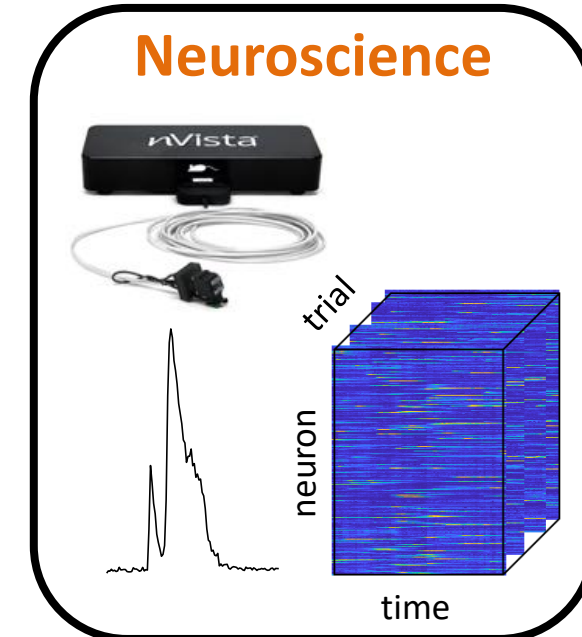
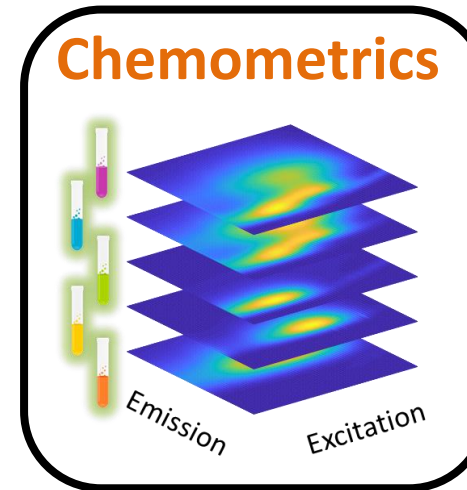


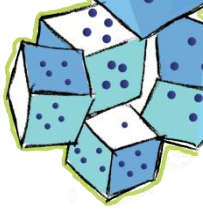


A moment for acknowledgment of greater issues

Tensors Come From Many Applications

- **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



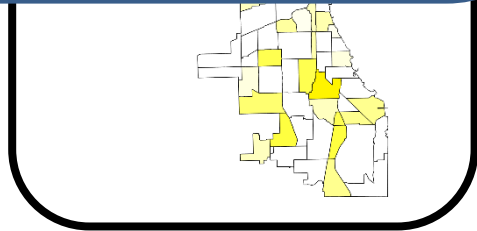


Tensors Come From Many Applications

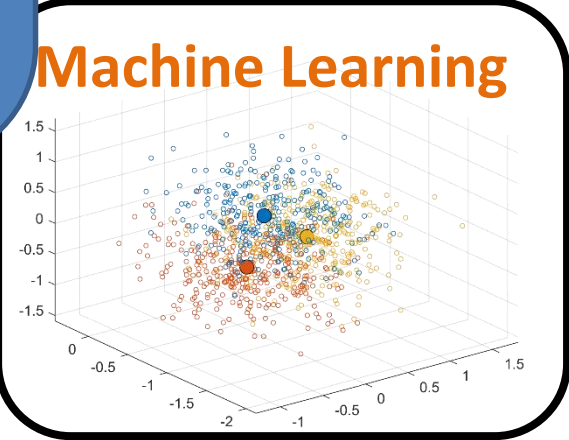
- **Chemometrics:** Emission x Excitation x Samples (Fluorescence Spectroscopy)
- **Neuroscience:** Neuron x Time x Trial
- **Criminology:** District x Crime Type x Time (Chicago Crime Data)
- **Machine Learning:** Mixture Models
- **Transportation:** Road Network x Time
- **Sports:** Player x Team x Time
- **Cyber-Traffic:** IP Address x Port x Time
- **Social Networks:** User x Interaction-Type x Time
- **Signal Processing:** Sensor x Frequency x Time
- **Trending Co-occurrence:** Term A x Term B x Time

Tensor Decomposition Finds Patterns in Massive Data (Unsupervised Learning)

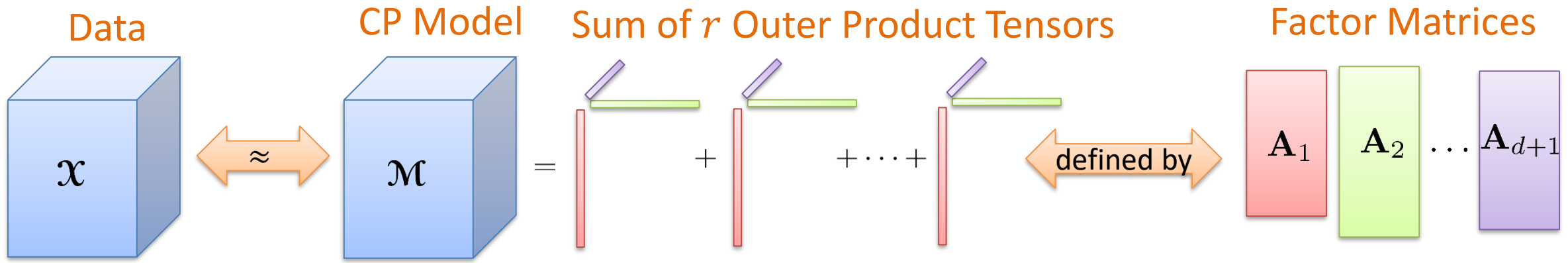
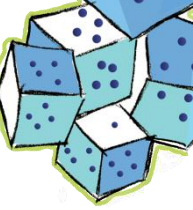
Chemometrics



Neuroscience



Tensor Decomposition Identifies Factors



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

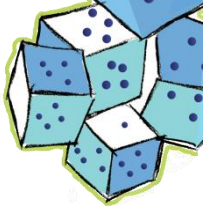
$$\mathcal{M} = [\mathbf{A}_1, \mathbf{A}_2, \dots, \mathbf{A}_{d+1}] \in \mathbb{R}^{n_1 \times n_2 \times \dots \times n_{d+1}}$$

$$\mathbf{A}_k \in \mathbb{R}^{n_k \times r}$$

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

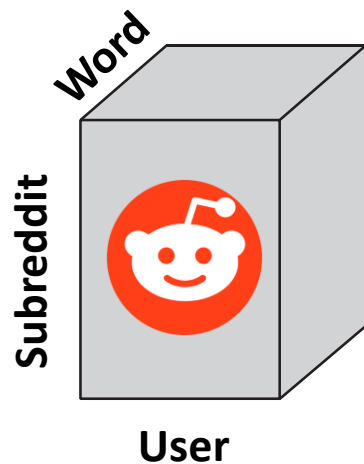
$$m_i = m(i_1, i_2, \dots, i_{d+1}) = \sum_{j=1}^r \prod_{k=1}^{d+1} a_k(i_k, j)$$

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://frostd.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 ($10^{-8}\%$)

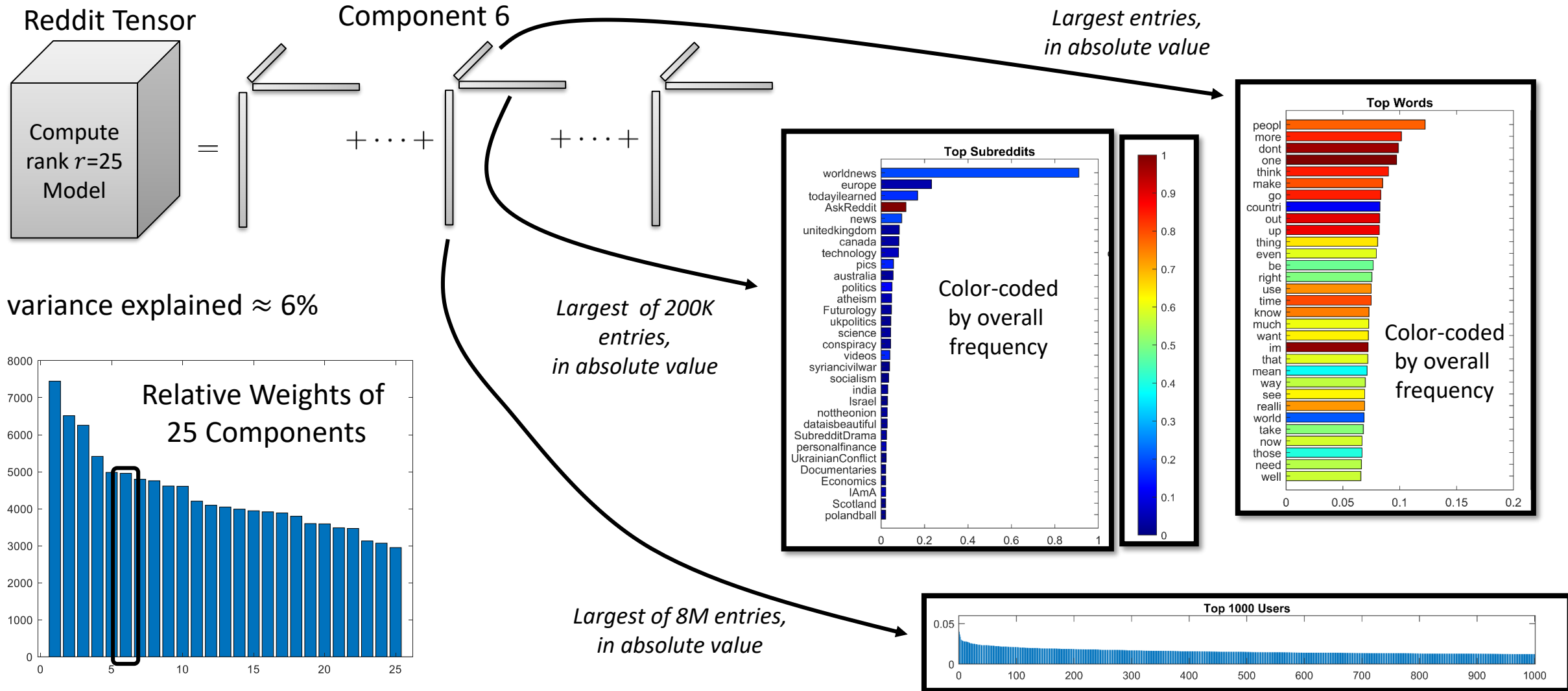
106 gigabytes

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

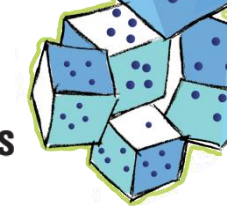
Used a rank $r = 25$ decomposition

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

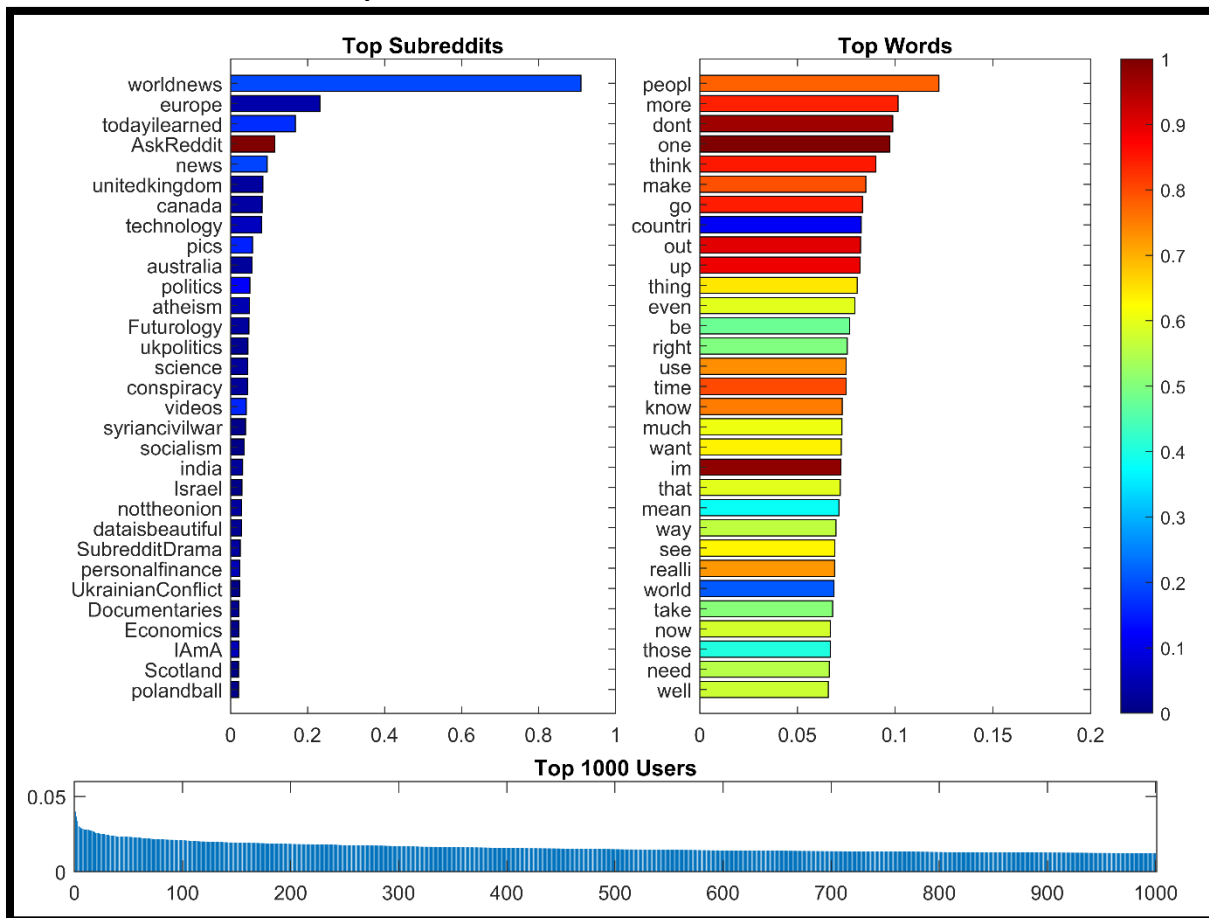
Interpreting Reddit Components



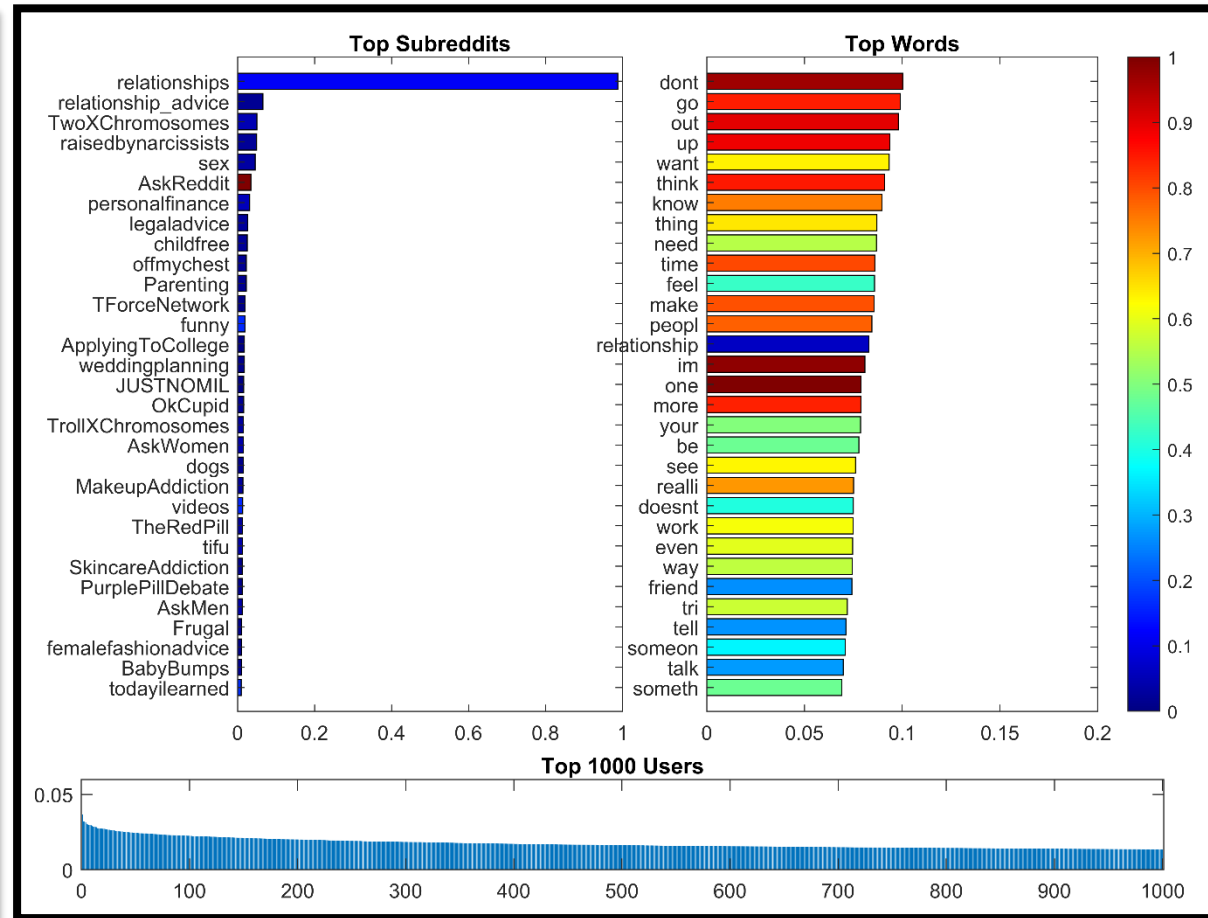
Example Reddit Components Include Rare Words Apropos to High-Scoring Reddits



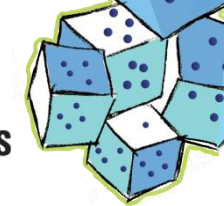
Component #6: International News



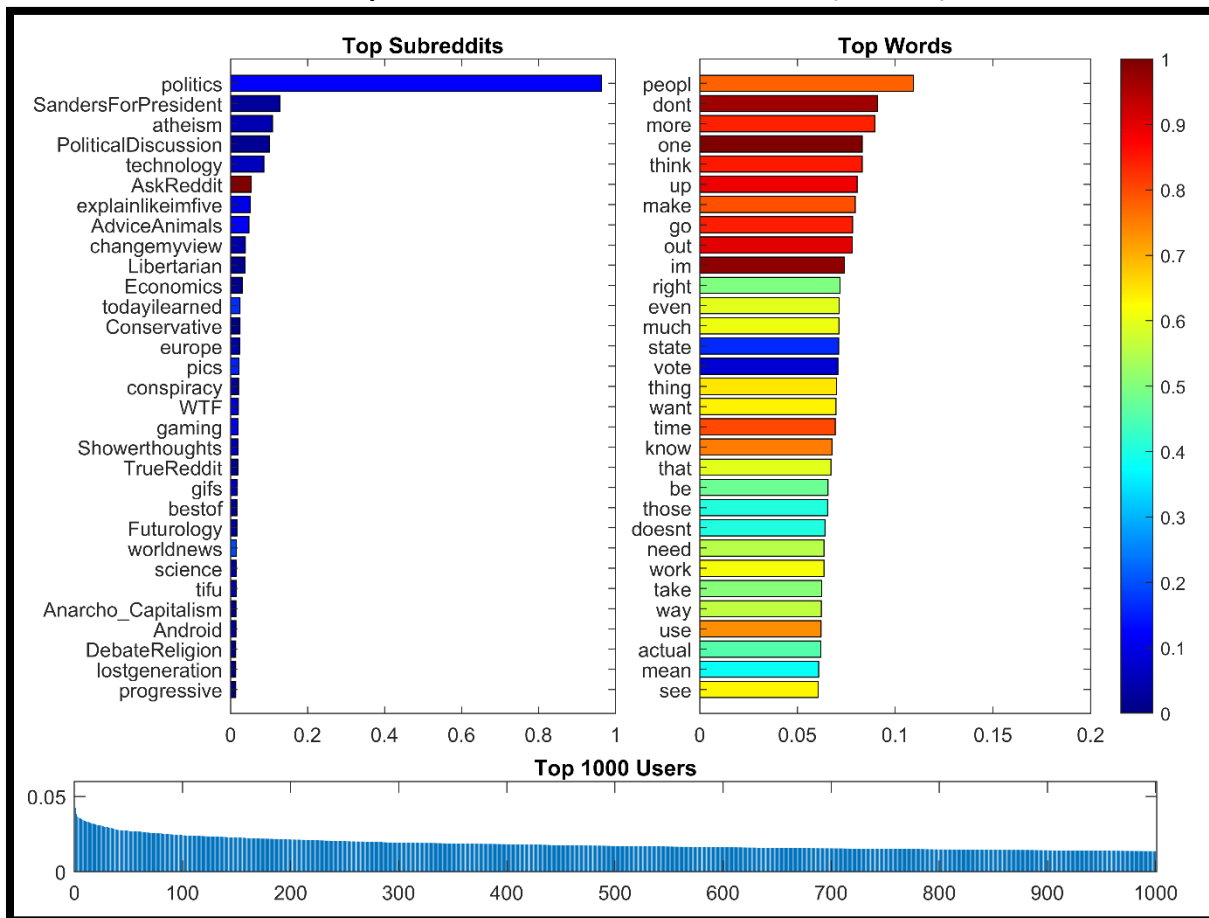
Component #8: Relationships



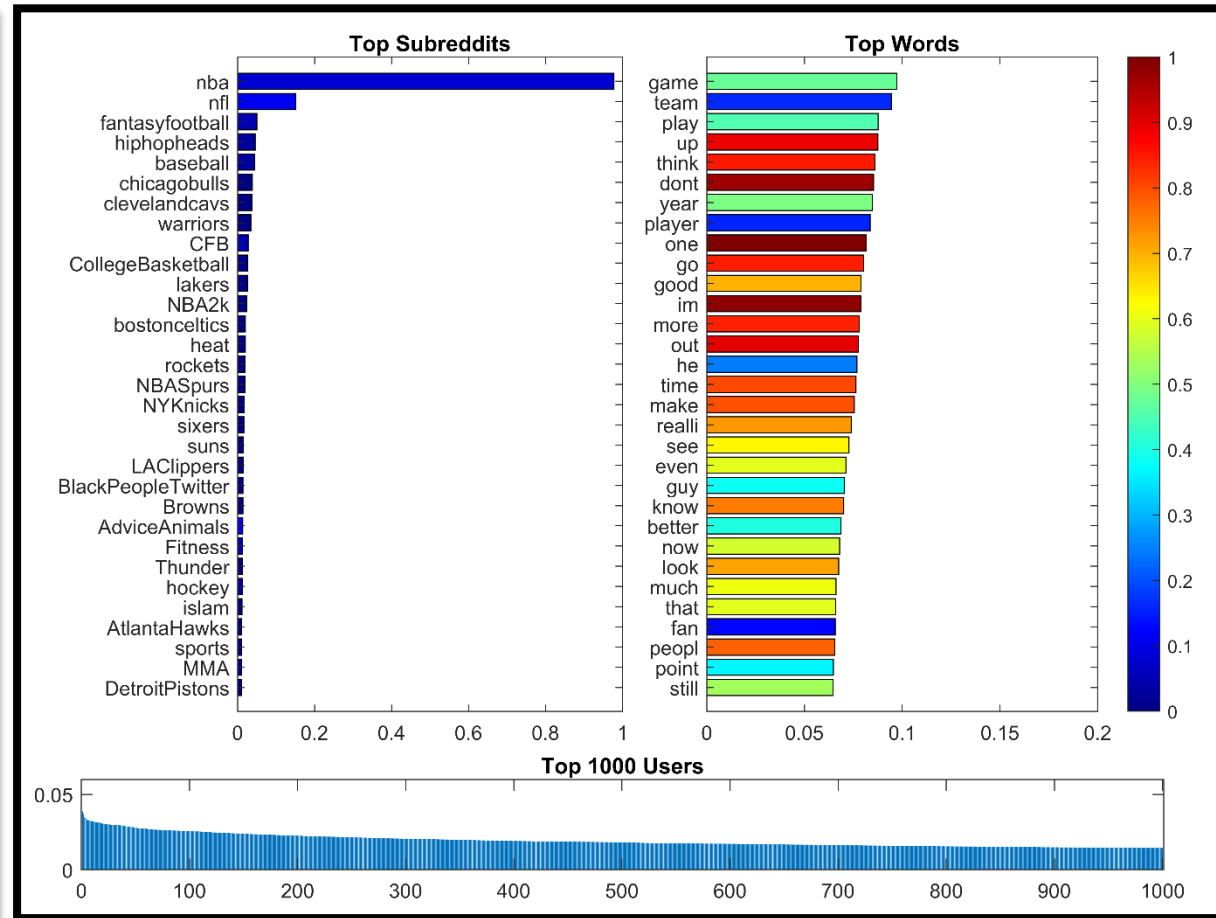
Example Reddit Components Include Rare Words Apropos to High-Scoring Reddits



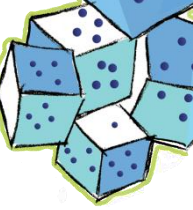
Component #9: U.S. Politics (2015)



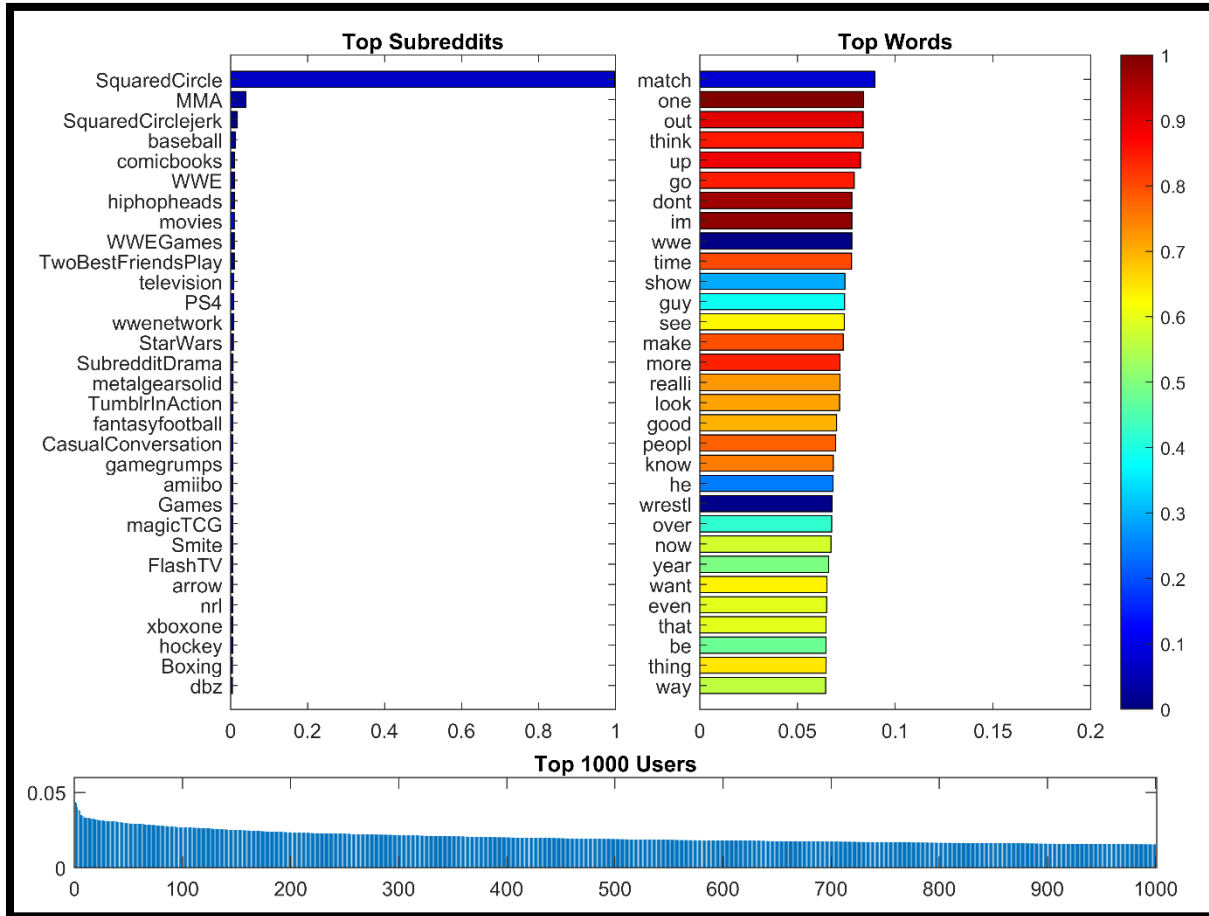
Component #11: Sports



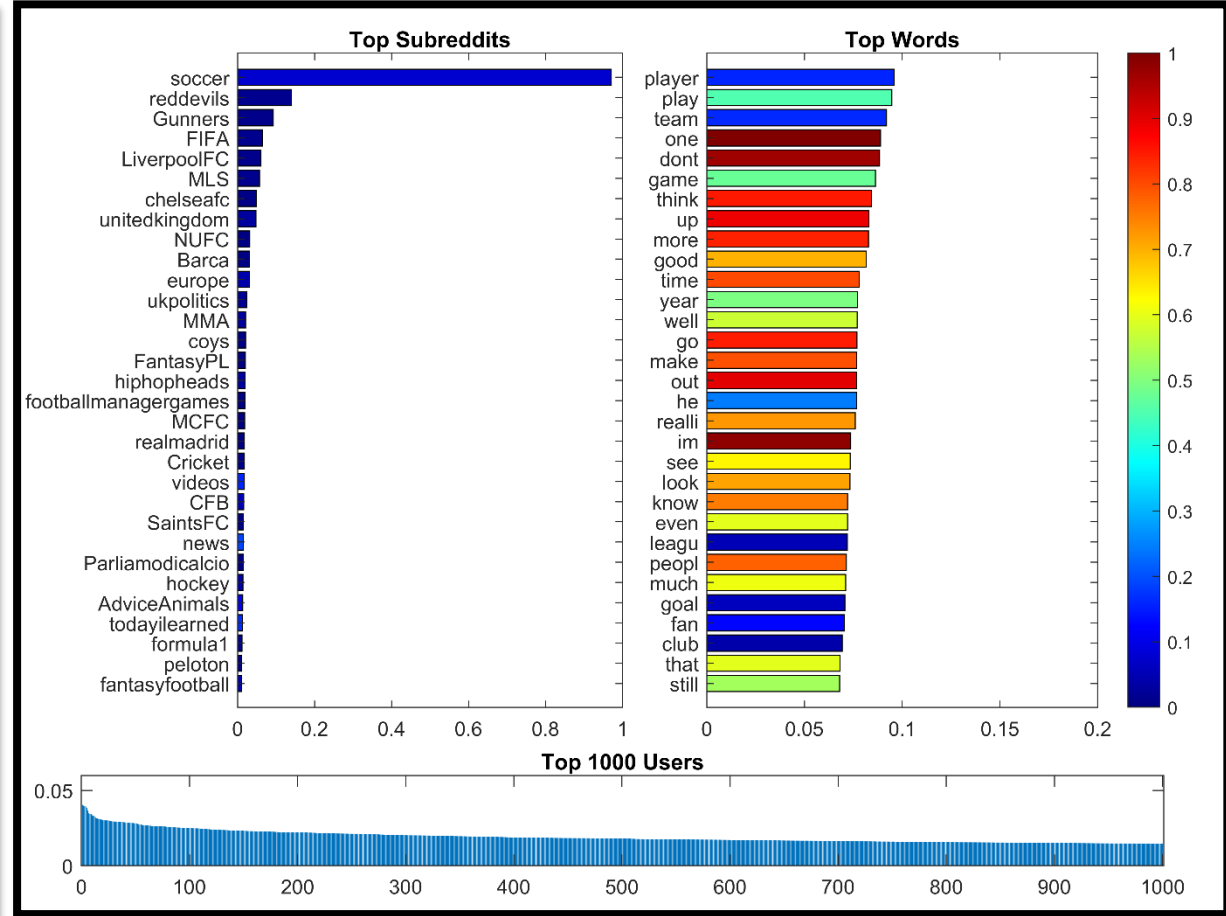
Example Reddit Components Include Rare Words Apropos to High-Scoring Reddits



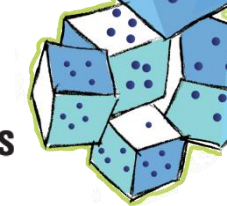
Component #15: Wrestling



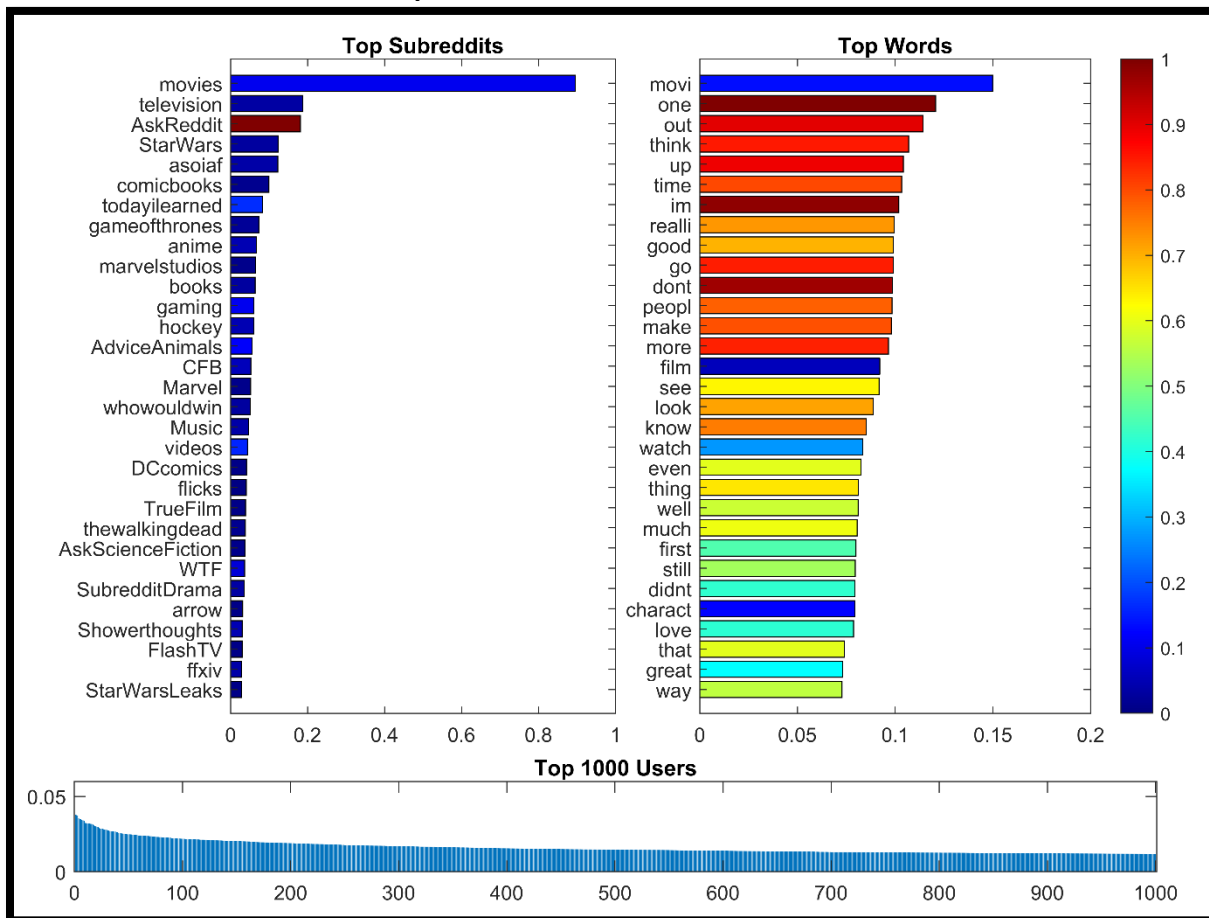
Component #18: Soccer



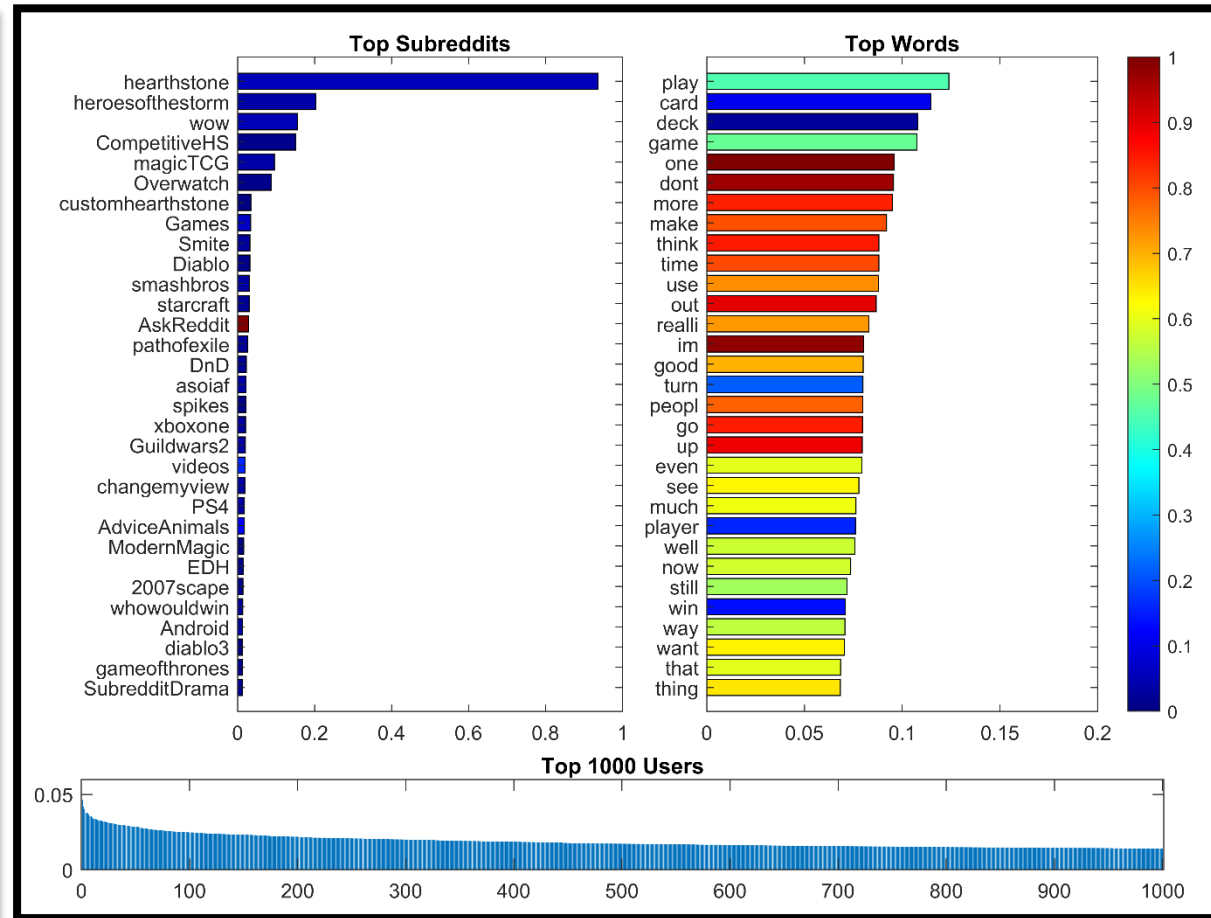
Example Reddit Components Include Rare Words Apropos to High-Scoring Reddits



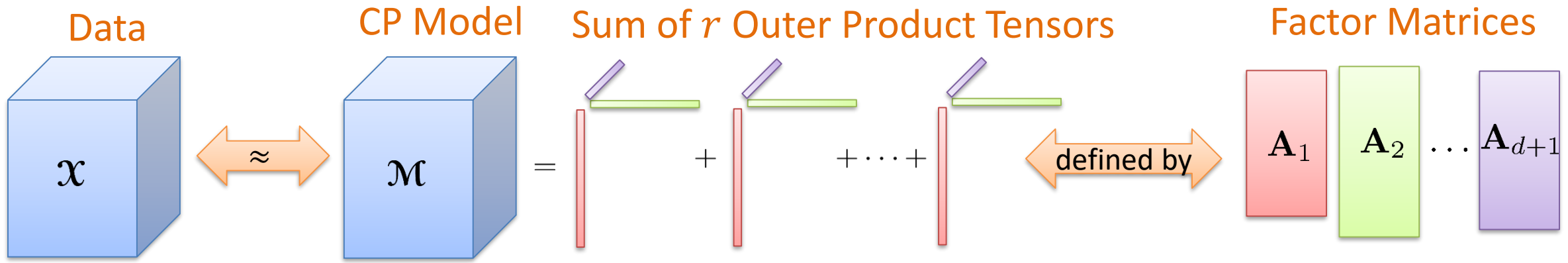
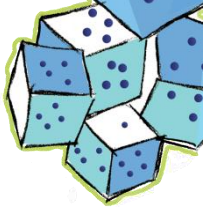
Component #19: Movies & TV



Component #18: Computer Card Game



Tensor Decomposition Identifies Factors



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

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

$$\mathbf{A}_k \in \mathbb{R}^{n_k \times r}$$

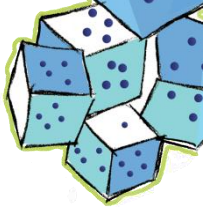
$$x_i = x(i_1, i_2, \dots, i_{d+1})$$

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

Model Rank

Key Idea: 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 Khatri-Rao Product (KRP) Structure



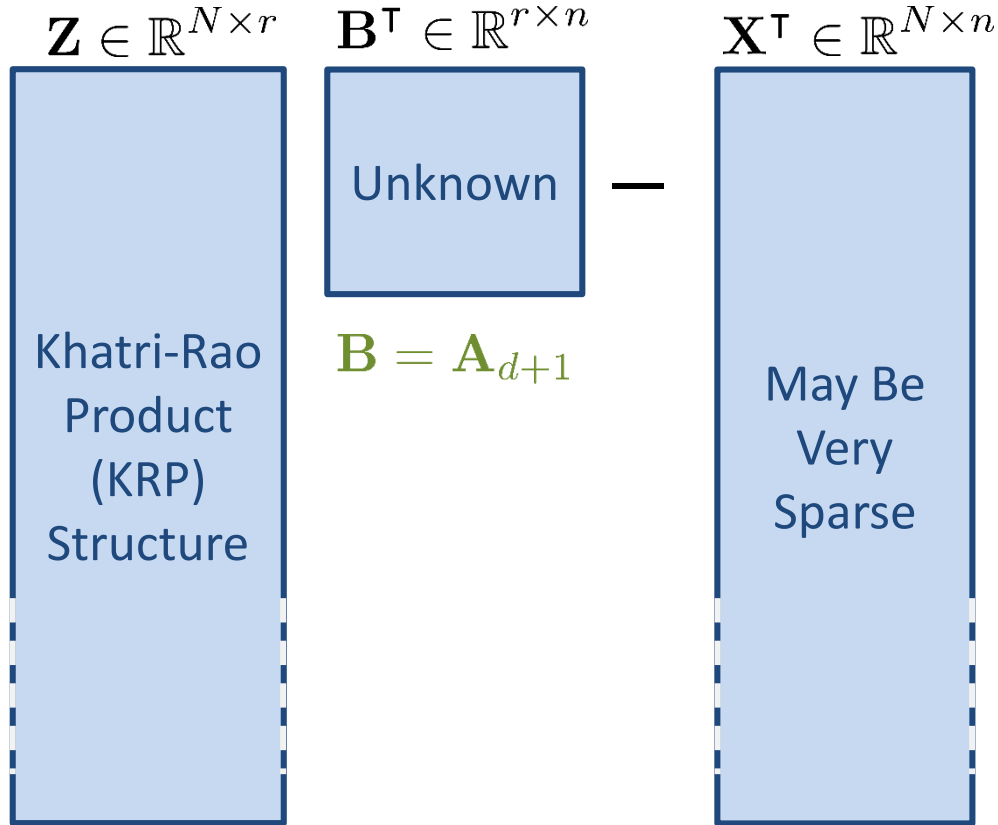
$$\min_{\mathbf{B}} \|\mathbf{Z}\mathbf{B}^T - \mathbf{X}^T\|^2$$

$$N \gg r, n$$

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

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

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

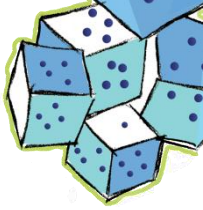


$$\mathbf{Z} = \mathbf{A}_d \odot \cdots \odot \mathbf{A}_1$$

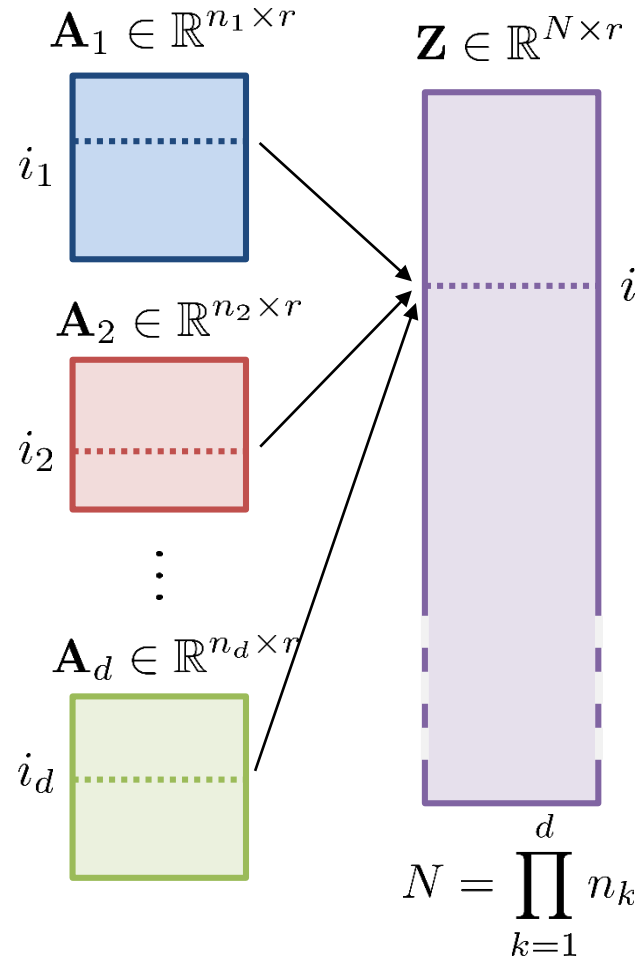
$$\mathbf{X} = \mathbf{X}_{(d+1)}$$

- 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 $O(r \text{ nnz}(\mathbf{X}))$

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:

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

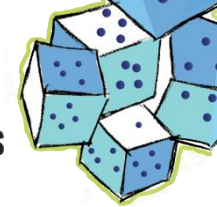
where

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

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

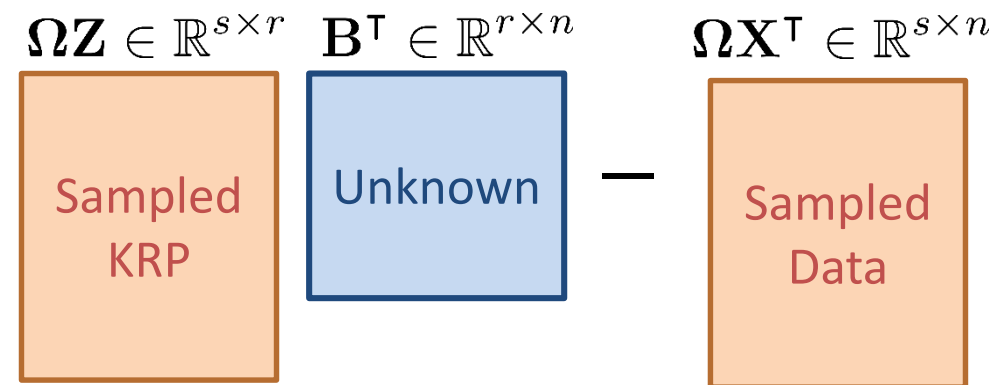
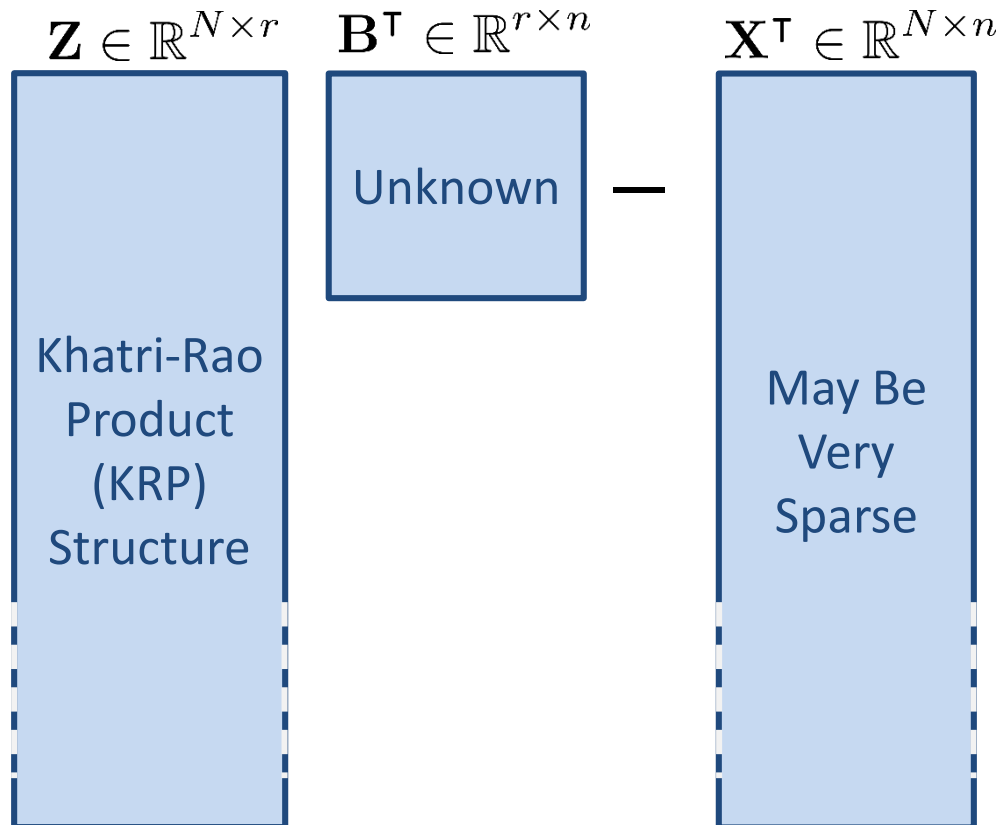
$$i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \cdots \otimes [n_d]$$

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



$$\min_{\mathbf{B}} \|\mathbf{ZB}^T - \mathbf{X}^T\|^2$$

$$\min_{\mathbf{B}} \|\Omega\mathbf{ZB}^T - \Omega\mathbf{X}^T\|^2$$



Complexity reduced from $O(Nnr)$ to $O(snr^2)$

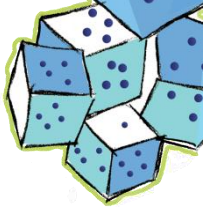
Key surveys:

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?

$$N \gg r, n$$

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



Probability distribution on rows of linear system

$$\sum_{i=1}^N p_i = 1$$

Not specifying yet how these probabilities are selected

Pick a **single** random index ξ with probability p_ξ

Choose

$$\Omega = \begin{bmatrix} 0 & \dots & 0 & \frac{1}{\sqrt{p_\xi}} & 0 & \dots & 0 \end{bmatrix} \in \mathbb{R}^{1 \times N}$$

\swarrow ξ th entry

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

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

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

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

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

Not specifying yet how s is determined

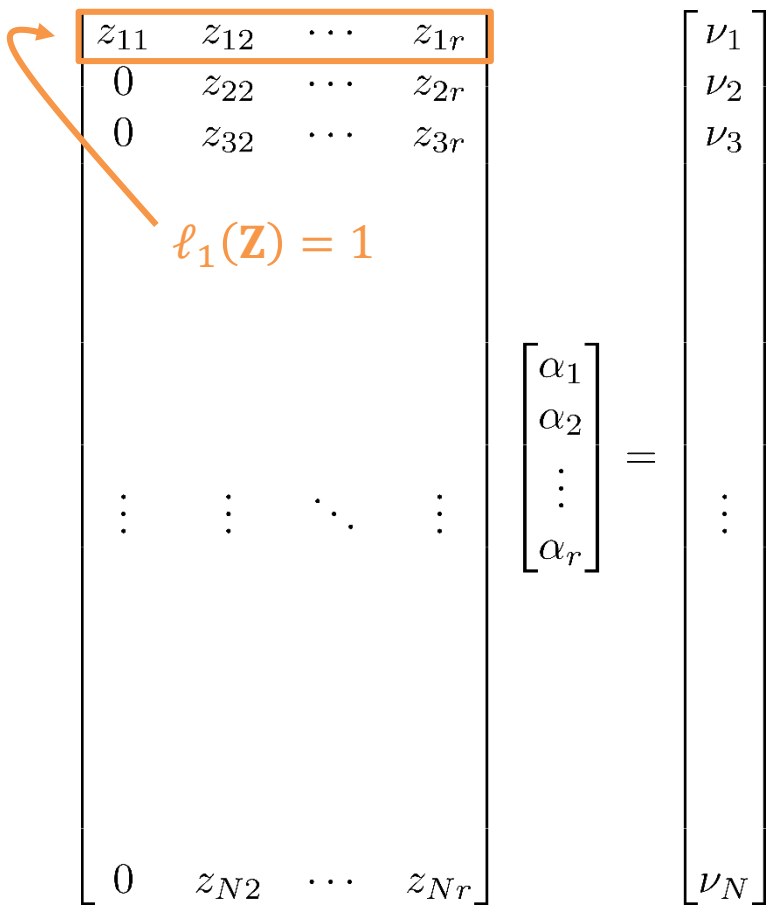
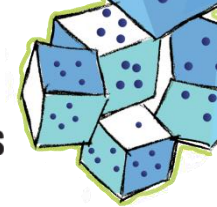
$$\omega(j, i) = \begin{cases} \frac{1}{\sqrt{s p_i}} & \text{if } \xi_j = i \\ 0 & \text{otherwise} \end{cases}$$

Each row has a single nonzero!

Then, as before, we have:

$$\mathbb{E} \|\Omega \mathbf{Z} \alpha - \Omega \nu\|^2 = \|\mathbf{Z} \alpha - \nu\|^2$$

Optimal Choice for Sampling Probability is Based on Leverage Scores



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

Leverage score:

Let \mathbf{Q} be any orthonormal basis of the column space of \mathbf{Z} .

Leverage score of row i :

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

Coherence:

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

$$r/N \leq \mu(\mathbf{Z}) \leq 1$$

Rough Intuition:

Key rows have high leverage score

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

where $\beta = \min_{i \in [N]} \frac{r p_i}{\ell_i(\mathbf{Z})}$

What if we do uniform sampling?

$$p_i = \frac{1}{N} \text{ for all } i \in [N],$$

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

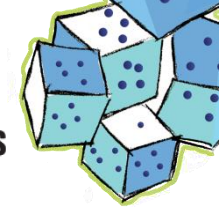
$$\Rightarrow \beta = 1 \Rightarrow s = O(\epsilon^{-2} \ln(r) r)$$

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

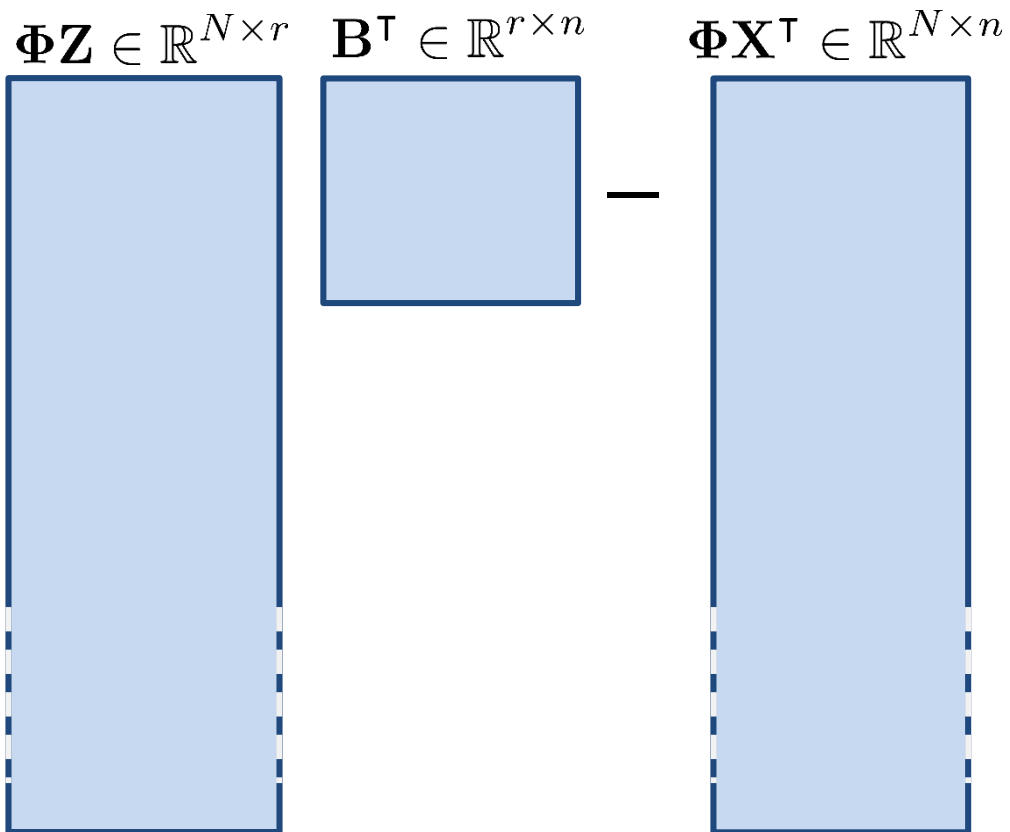
$$\Rightarrow \beta = r/N \Rightarrow s = O(\epsilon^{-2} \ln(r) N)$$

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

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

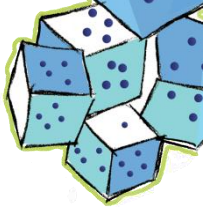


Transform System: $\min_{\mathbf{B} \in \mathbb{R}^{r \times n}} \|\Phi \mathbf{Z} \mathbf{B}^T - \Phi \mathbf{X}\|_F^2$

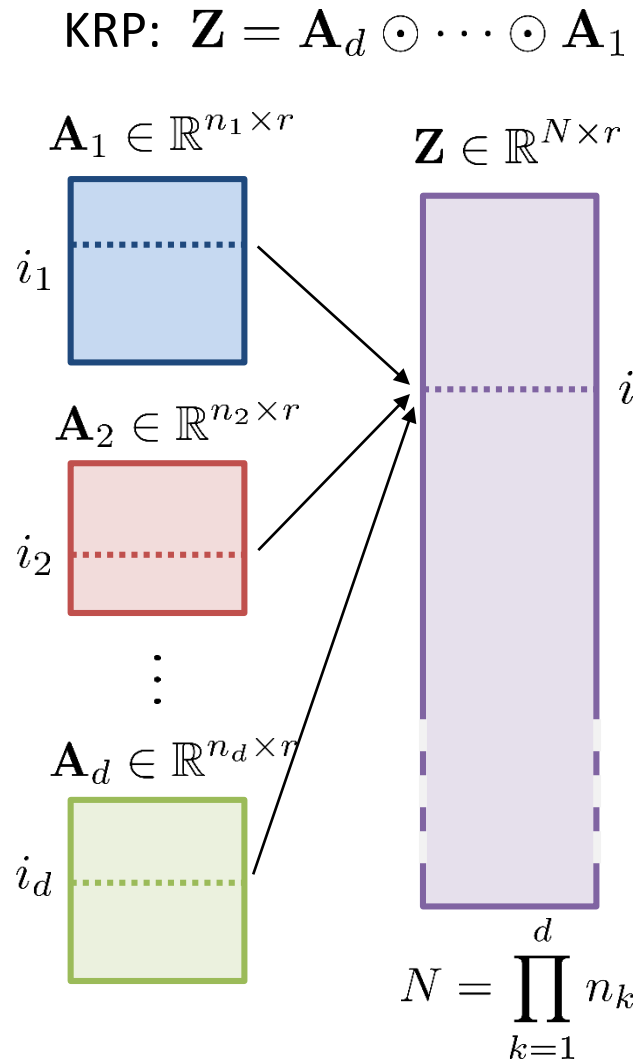


$$N \gg r, n$$

- Choose Φ so that all leverage scores of $\Phi \mathbf{Z}$ 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 \mathbf{Z}
 - Sample rows of \mathbf{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 #3: Bound Leverage Scores



Upper Bound on Leverage Score

Lemma (Cheng et al., NIPS 2016; Battaglino et al., SIMAX 2018):

$$l_i(\mathbf{Z}) \leq \prod_{k=1}^d l_{i_k}(\mathbf{A}_k)$$

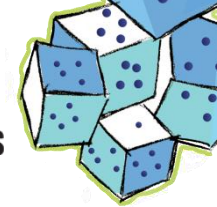
Too expensive to calculate $O(Nr^2)$

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

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

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

Ingredient #4: Use Factor Matrix Leverage Scores for Sampling Probabilities (Main Thm)



Given linear system: $\|\mathbf{ZB}^\top - \mathbf{X}^\top\|^2$ with $\mathbf{Z} = \mathbf{A}_d \odot \dots \odot \mathbf{A}_1 \in \mathbb{R}^{N \times r}$, $\mathbf{X}^\top \in \mathbb{R}^{n \times N}$

Define sampling probabilities:

$$p_i = \frac{1}{r^d} \prod_{k=1}^d \ell_{i_k}(\mathbf{A}_k) \text{ for all } i \in [N]$$

Leverage Scores

$$\ell_{i_k}(\mathbf{A}_k) = \|\mathbf{Q}_k(i_k, :)\|_2 \text{ where } \mathbf{Q}_k \text{ is orthonormal basis for column space of } \mathbf{A}_k$$

And random sampling matrix:

Pick a s random indices ξ_j such that $P(\xi_j = i) = p_i$ and define

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

Solve sampled problem:

$$\tilde{\mathbf{B}}_* \equiv \arg \min_{\mathbf{B} \in \mathbb{R}^{r \times n}} \|\Omega \mathbf{ZB}^\top - \Omega \mathbf{X}\|_F^2$$

Get probabilistic error bound:

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

$$\|\mathbf{Z}\tilde{\mathbf{B}}_*^\top - \mathbf{X}^\top\|_F^2 \leq (1 + O(\epsilon)) \|\mathbf{ZB}_*^\top - \mathbf{X}^\top\|_F^2$$

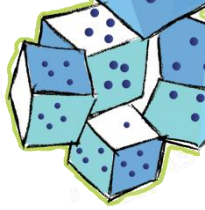
when number of samples satisfies:

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

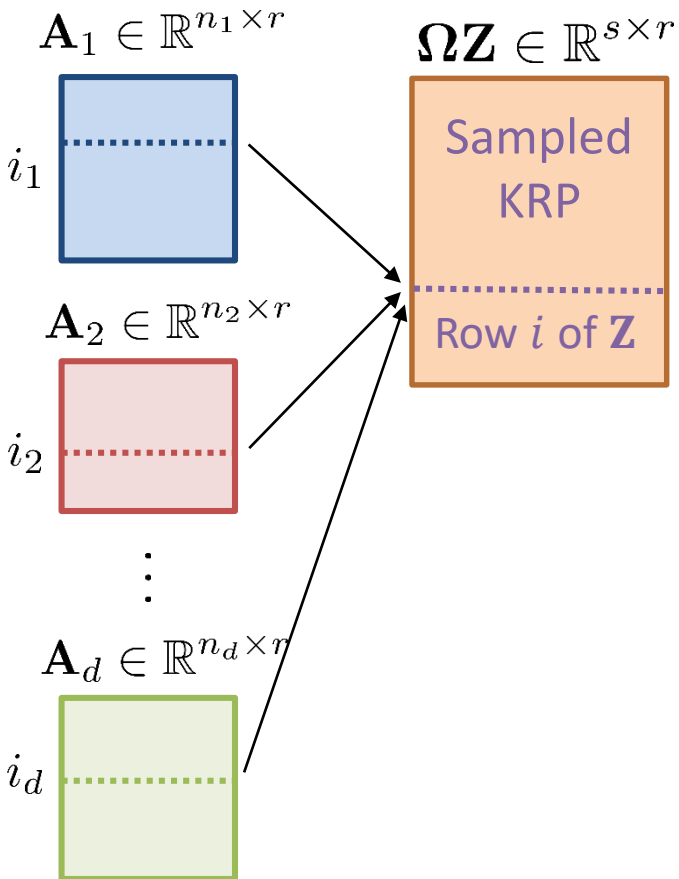
1-1 Correspondence between linear index and multi index:

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

Ingredient #5: Efficient Sampling without Forming KRP



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



Upper Bound on Leverage Score

Lemma (Cheng et al., NIPS 2016; Battaglino et al., SIMAX 2018):

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

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

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

Recall probability of sampling row i

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

But still don't want to consider all N possible combinations corresponding to all rows of \mathbf{Z} !

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

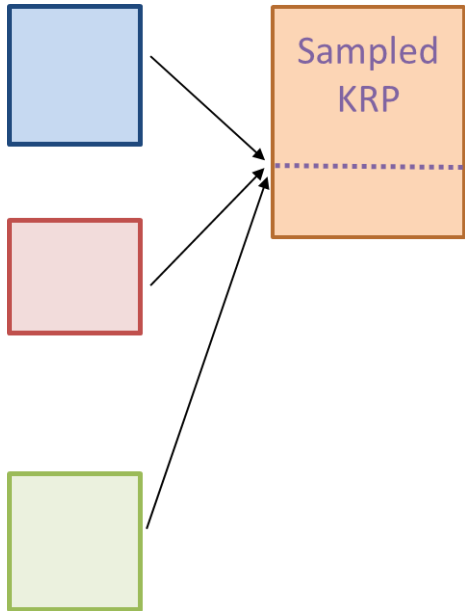
$$i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \cdots \otimes [n_d]$$

Ingredient #6: Combine Repeated Rows

Problem: Concentrated sampling probabilities identify a few key rows *but* can lead to *many* repeats!

Least Squares Problems from Real-world Tensor Data Sets

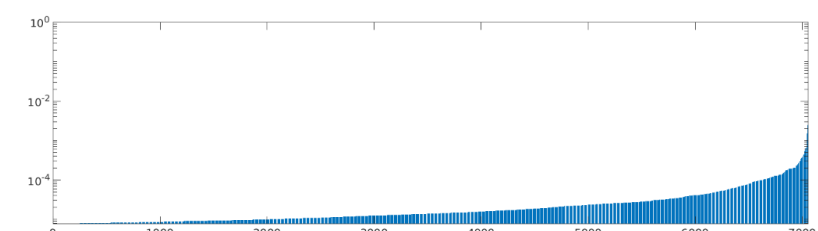
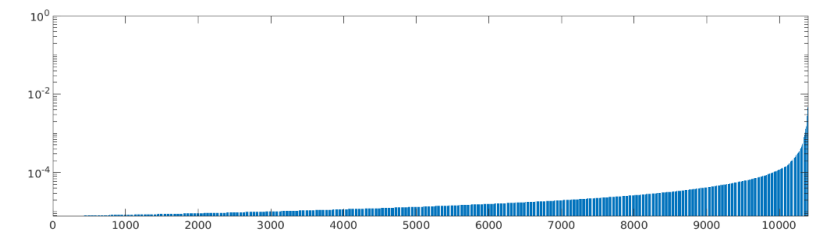
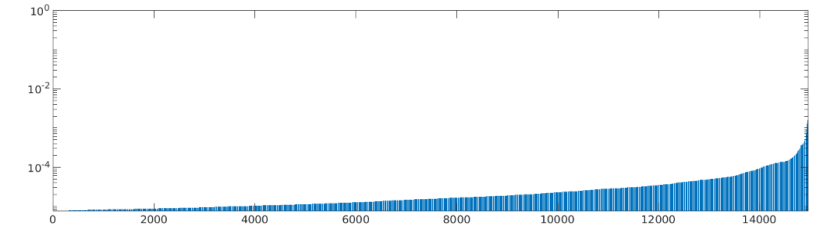
Combining repeat rows \Rightarrow 2-20X speedup



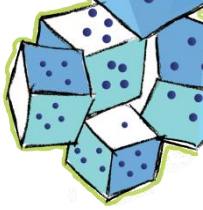
Example 1: $N = 3.2e12, s = 2^{17}, \tau = \frac{1}{s} = 8e-6$
 $\mathcal{D} = \{i : p_i > \tau\}, |\mathcal{D}| \approx 15000, \sum_{i \in \mathcal{D}} p_i = 0.51$

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: $N = 8.6e12, s = 2^{17}, \tau = \frac{1}{s} = 8e-6$
 $\mathcal{D} = \{i : p_i > \tau\}, |\mathcal{D}| \approx 7000, \sum_{i \in \mathcal{D}} p_i = 0.25$



Ingredient #7: Hybrid Deterministic and Randomly-Sampled Rows



Deterministic Rows

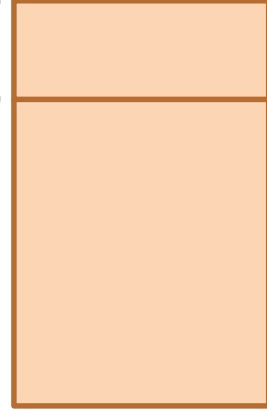
$$\mathcal{D}_\tau = \{i \in [N] \mid p_i \geq \tau\}$$

$$s_{\text{det}} = |\mathcal{D}_\tau|$$

$$p_{\text{det}} = \sum_{i \in \mathcal{D}_\tau} p_i$$

```
for  $i \in \mathcal{D}_\tau$  do
  add row  $\mathbf{A}_1(i_1, :) * \dots * \mathbf{A}_d(i_d, :)$ 
end for
```

$$\Omega \mathbf{Z} \in \mathbb{R}^{s \times r}$$



Random Rows

$$s_{\text{rnd}} = s - s_{\text{det}}$$

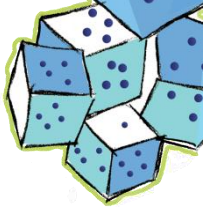
```
for  $j = 1 \dots, s_{\text{rnd}}$  do
  repeat
    for  $k = 1 \dots, d$  do
       $i_k \leftarrow \text{multi}(\ell(\mathbf{A}_k)/r)$ 
    end for
  until  $i \notin \mathcal{D}_\tau$ 
   $\omega \leftarrow \sqrt{(1 - p_{\text{det}})/(s_{\text{rnd}} p_i)}$ 
  add row  $\omega (\mathbf{A}_1(i_1, :) * \dots * \mathbf{A}_d(i_d, :))$ 
end for
```

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

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

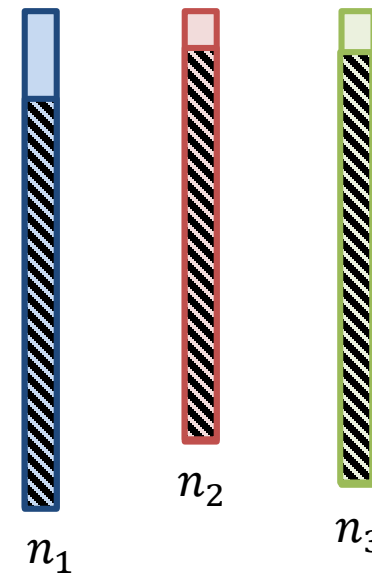
$$p_i \equiv \frac{1}{r^d} \prod_{k=1}^d \ell_{i_k}(\mathbf{A}_k)$$

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

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

- 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

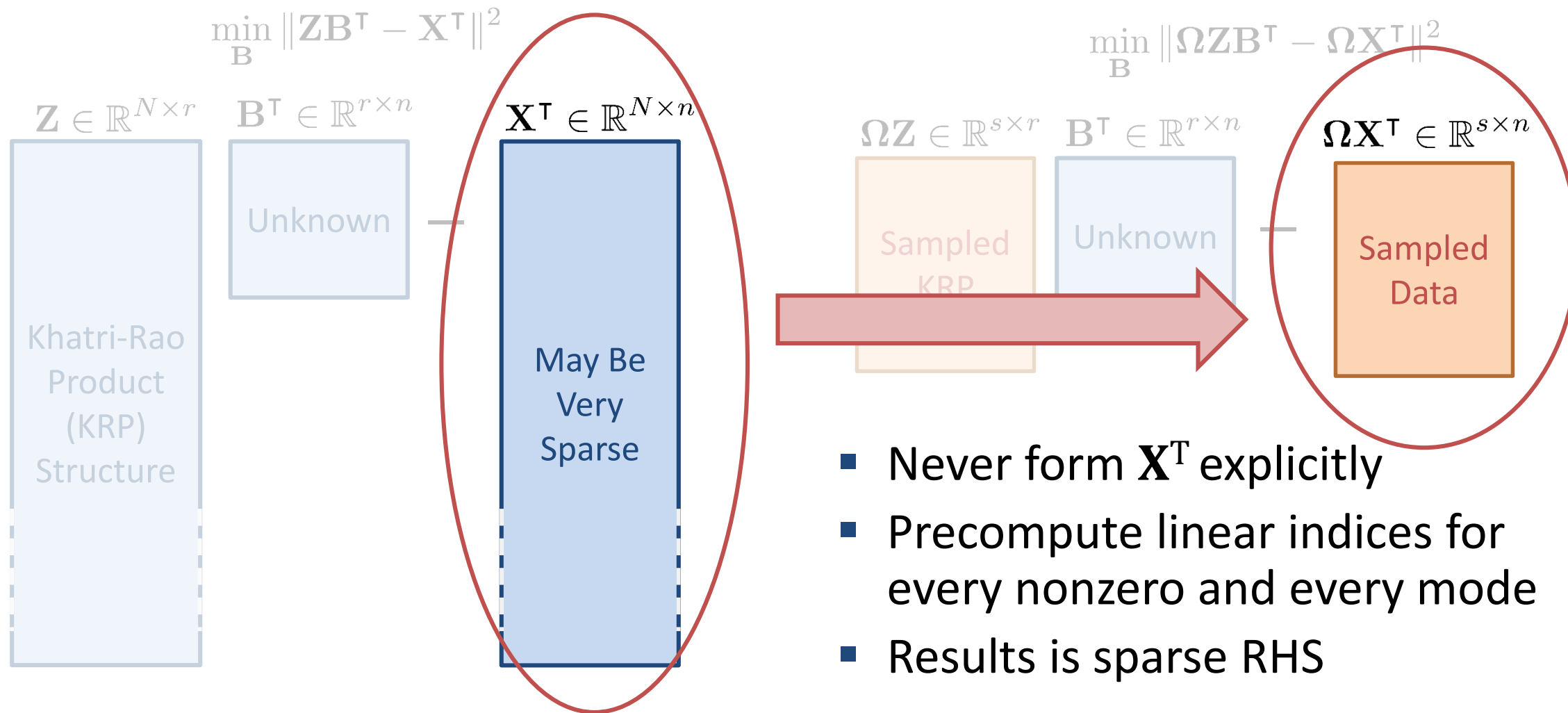
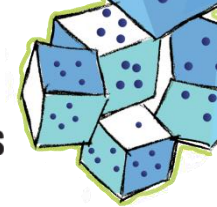
Sorted Leverages Scores (Descending)



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

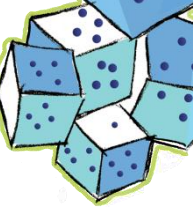
$$i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \dots \otimes [n_d]$$

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



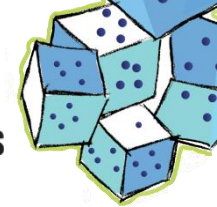
- Never form X^T explicitly
- Precompute linear indices for every nonzero and every mode
- Results is sparse RHS

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

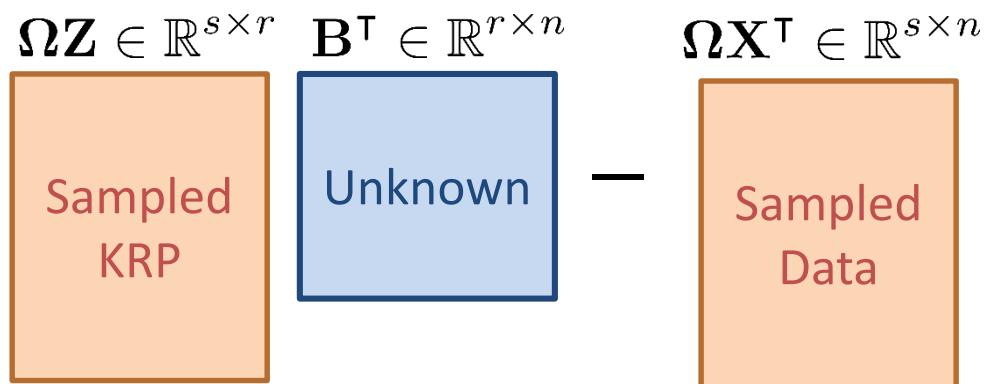


Numerical Results

Solution Quality as Number of Samples Increase and Hybrid Improvements



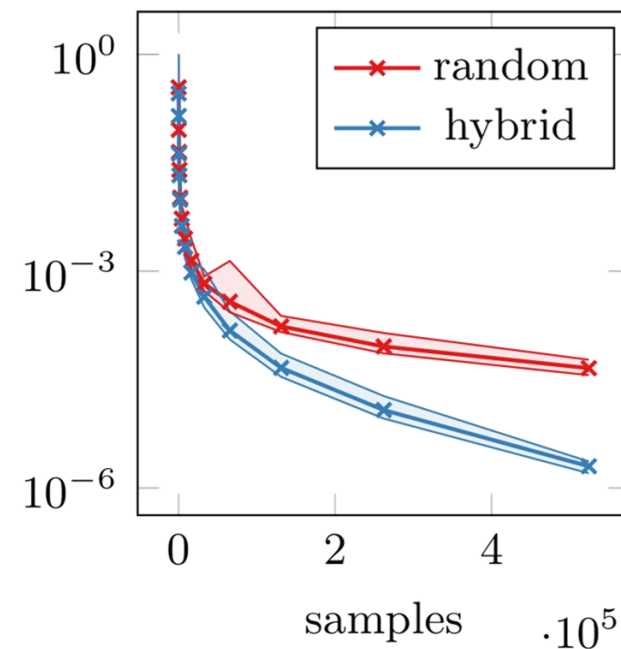
Single Least Squares Problem with $N = 46M$ rows, $r = 10$ columns, $n = 183$ right-hand sides



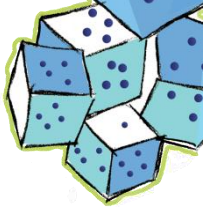
$$\tilde{\mathbf{B}}_* \equiv \arg \min_{\mathbf{B} \in \mathbb{R}^r} \|\Omega \mathbf{Z} \mathbf{B}^T - \Omega \mathbf{X}^T\|_2^2$$

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

$$\frac{\left| \|\mathbf{Z} \mathbf{B}_*^T - \mathbf{X}^T\|_2 - \|\mathbf{Z} \tilde{\mathbf{B}}_*^T - \mathbf{X}^T\|_2 \right|}{\max \{ 1, \|\mathbf{Z} \mathbf{B}_*^T - \mathbf{X}^T\|_2 \}}$$

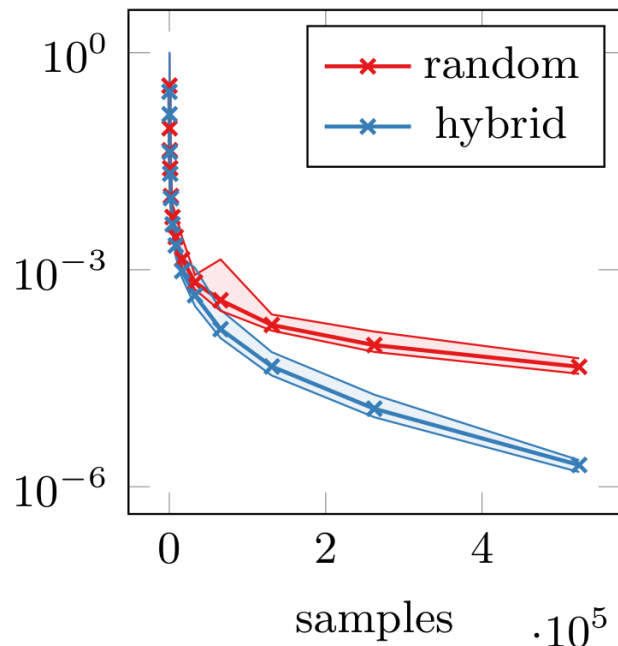


Deterministic Can Account for Substantial Portion of Probability

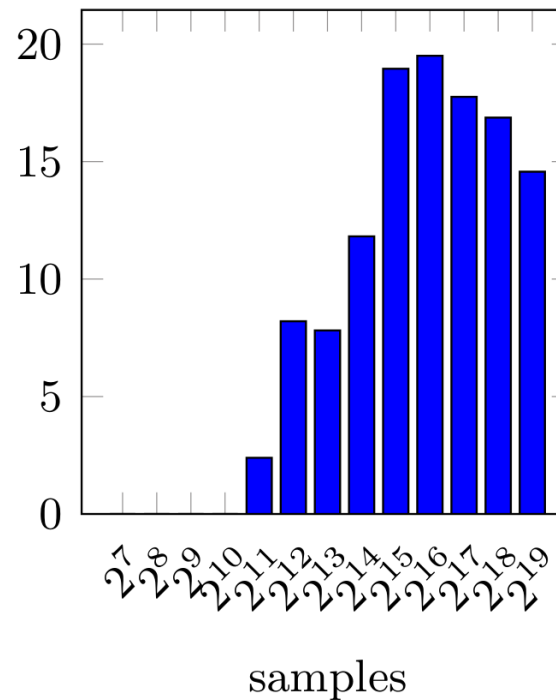


Single Least Squares Problem with $N = 46M$ rows, $r = 10$ columns, $n = 183$ right-hand sides

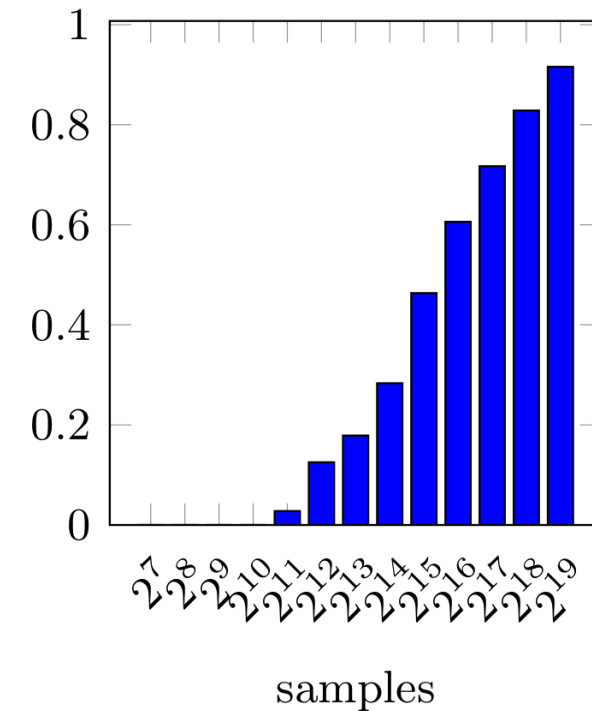
Difference to True Residual



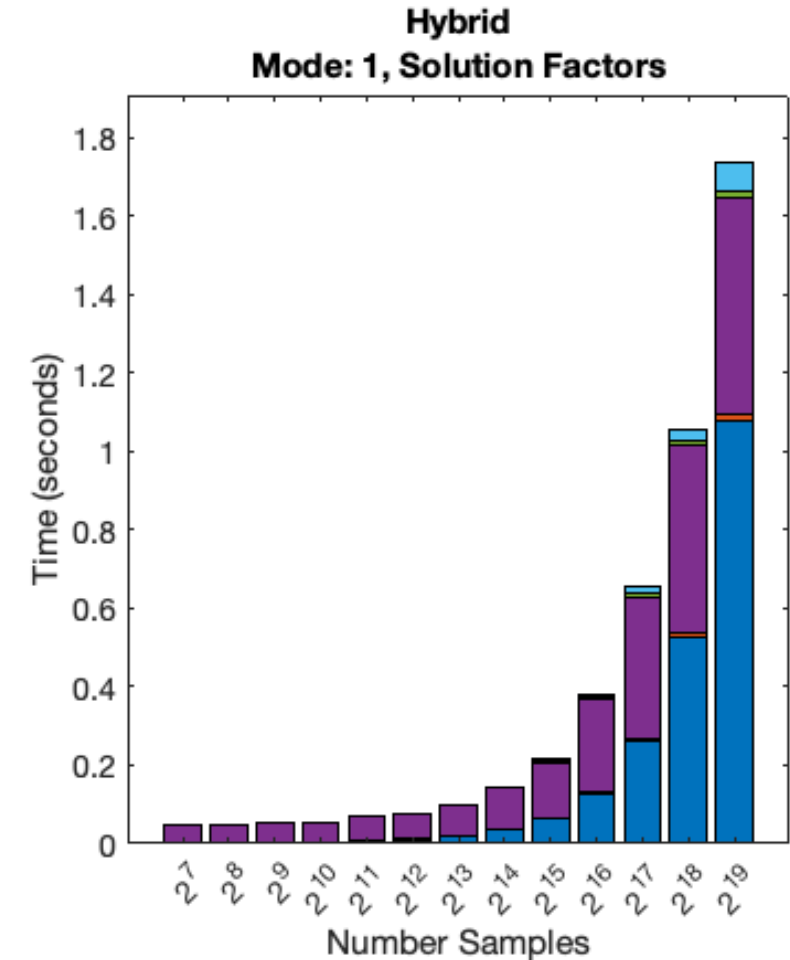
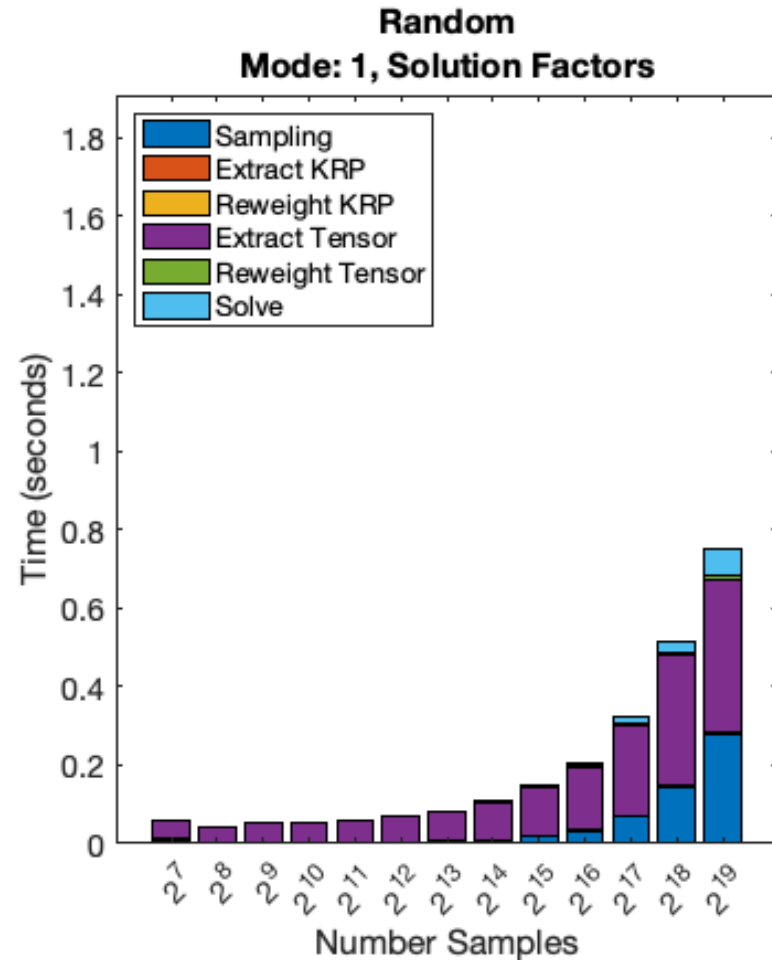
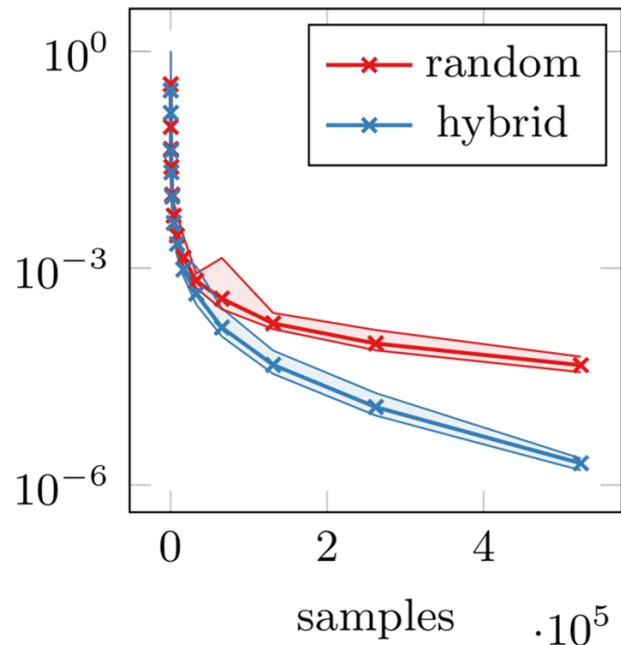
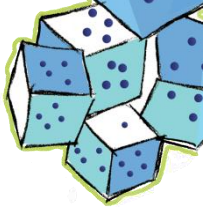
Percent Above $\tau (s_{det}/s)$



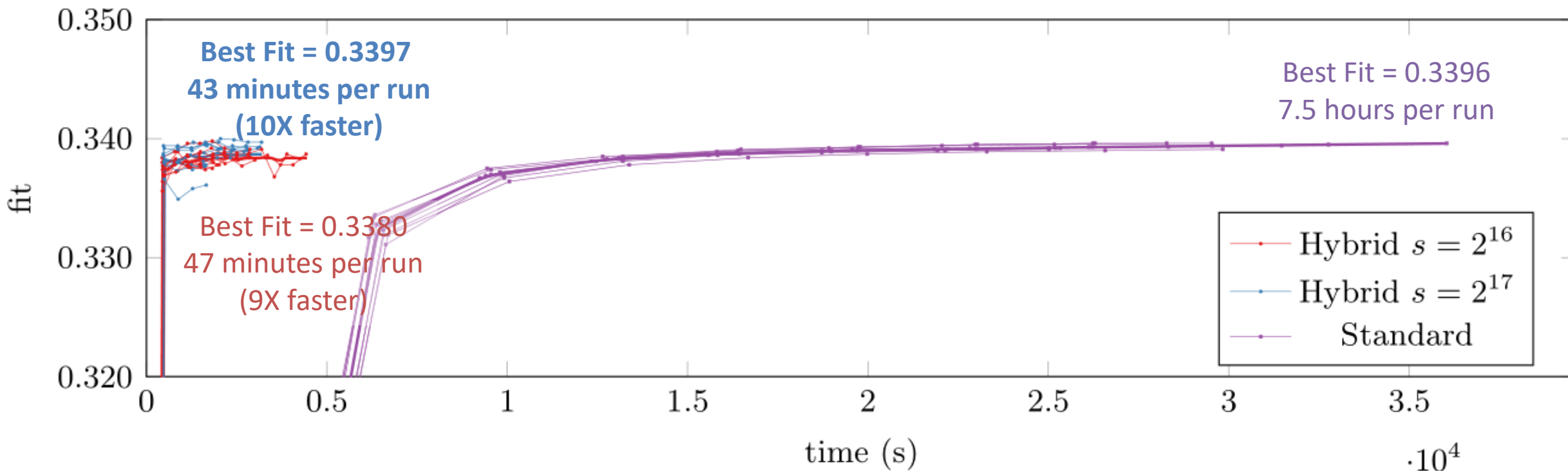
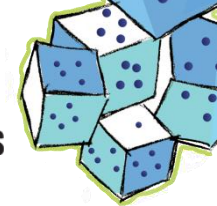
p_{det}



Some Trade-off Between Accuracy and Expense for Deterministic

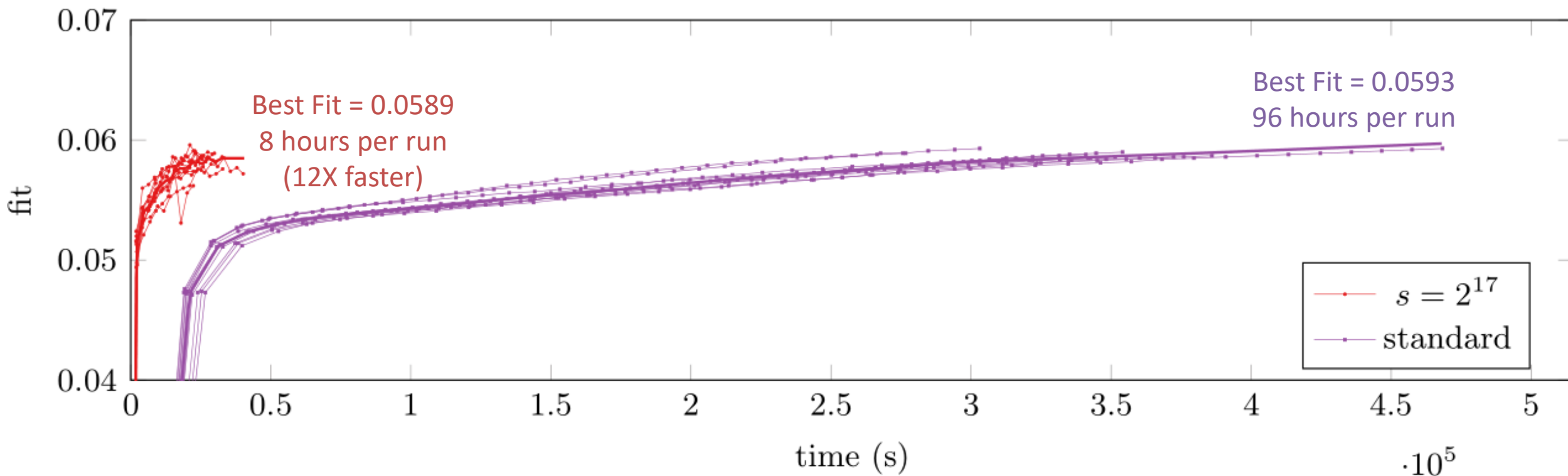
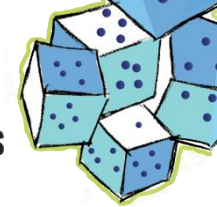


Over 9X Speed-up for Amazon Tensor with 1.7 Billion Nonzeros

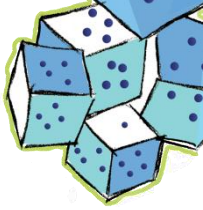


Amazon Tensor: 4.8M x 1.8M x 1.8M Amazon Tensor with 1.7B nonzeros.
Rank $r = 25$ CP decomposition

Over 12X Speed-up for Reddit Tensor with 4.7 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

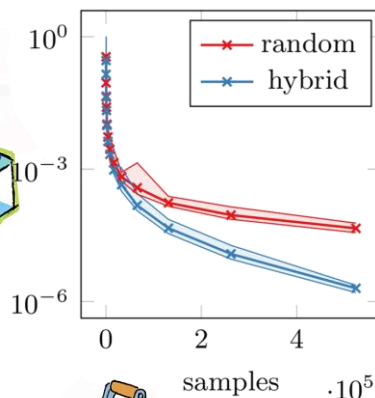


Conclusions & Future Work

- How to make CP tensor decomposition faster for large-scale 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? Pre-compute 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.

Larsen and Kolda,
*Practical Leverage-Based
Sampling for Tensor
Decomposition*,
arXiv:2006.16438, 2020

Difference to True Residual



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