

Practical Leverage-Based Sampling for Low-Rank Tensor Decomposition

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Joint work with Brett Larsen Stanford University

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Ilustration by Chris Brigmar



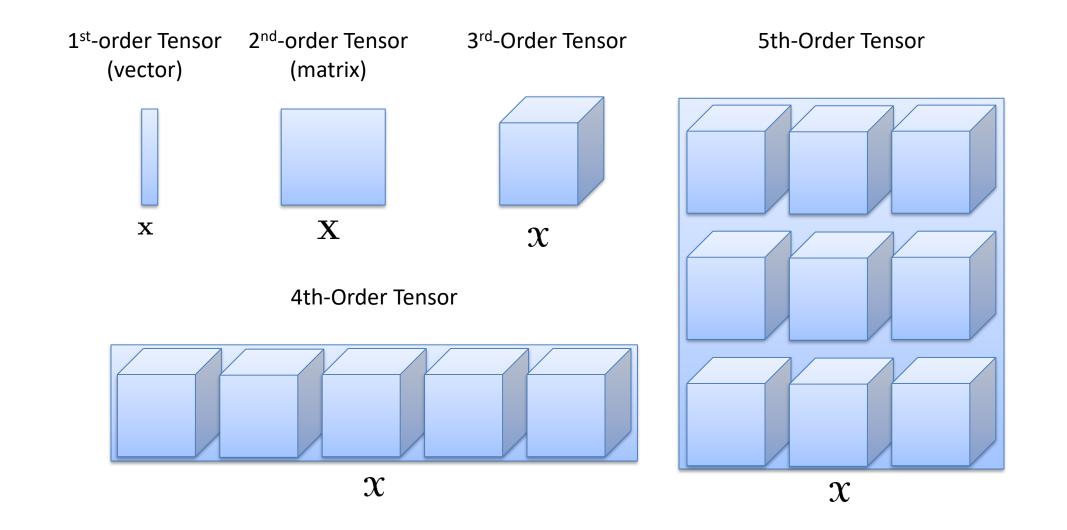


Funding & Reference

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- Brett was also funded by DOE Computational Science Graduate Fellowship (CSGF), administered by the Krell Institute
- B. W. Larsen, T. G. Kolda. Practical Leverage-Based Sampling for Low-Rank Tensor Decomposition. arXiv:2006.16438,2020. <u>http://arxiv.org/abs/2006.16438</u>

A Tensor is an Multi-Way Array

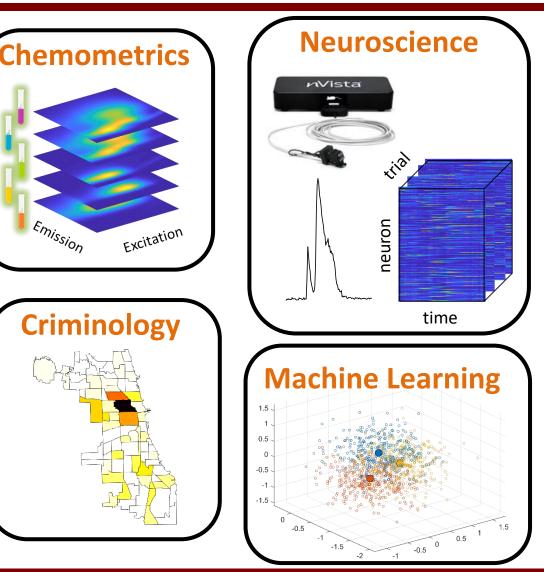






Tensors Come From Many Applications

- 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

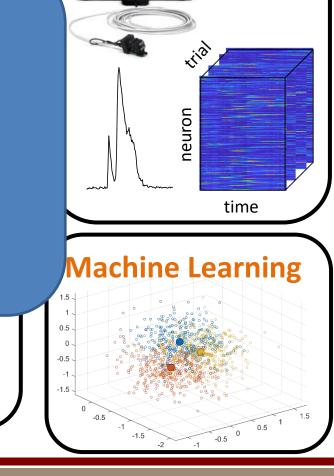


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Tensor Decomposition Finds Patterns in Massive Data (Unsupervised Learning)

Chemometrics



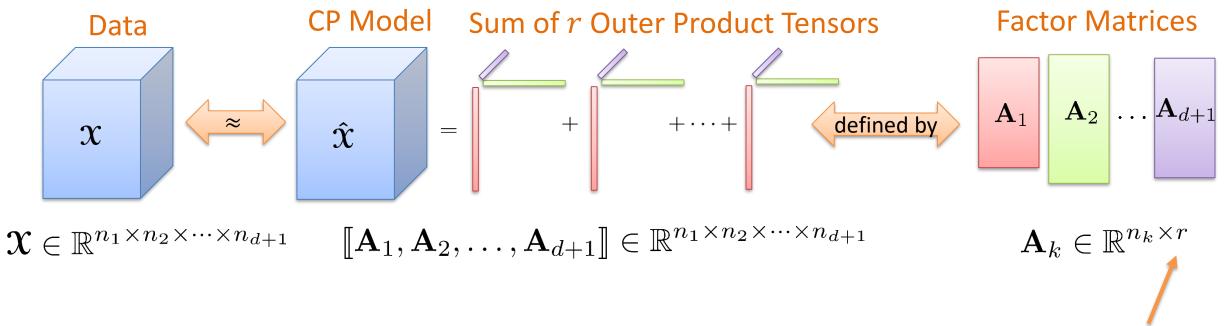
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Neuroscience

nVista



Tensor Decomposition Identifies Factors



10/6/2020

Frank Lauren Hitchcock

MIT Professor

(1875 - 1957)

CP First Invented in 1927

THE EXPRESSION OF A TENSOR OR A POLYADIC AS A SUM OF PRODUCTS

By FRANK L. HITCHCOCK

1. Addition and Multiplication.

Tensors are added by adding corresponding components. The product of a covariant tensor $A_{i_1 \dots i_n}$ of order p into a covariant tensor $B_{i_{n+1}} \dots i_{n+q}$ of order q is defined by writing

$$\mathbf{A}_{i_1\cdots i_p}\mathbf{B}_{i_{p+1}\cdots i_{p+q}} = \mathbf{C}_{i_1\cdots i_{p+q}} \tag{1}$$

where the product $C_{i_1 \dots i_{p+q}}$ is a covariant tensor of order p+q. When no confusion results indices may be omitted giving AB = C

equivalent to the n^{p+q} equations (1). Boldface type is convenient for indicating that the letters do not denote merely numbers or scalars. Products of contravariant and of mixed tensors may be similarly defined.

A partial statement of the problem to be considered is as follows: to find under what conditions a given tensor can be expressed as a sum of products of assigned form. A more general statement of the problem will be given below.

2. Polyadic form of a tensor.

Any covariant tensor $A_{i_1 \dots i_p}$ can be expressed as the sum of a finite number of tensors each of which is the product of p covariant vectors,

$$A_{i_{1}} \dots i_{p} = \sum_{j=1}^{j=h} a_{lj, i_{1}} a_{2j, i_{2}} \cdots a_{pj, i_{p}}$$
(2)

where a_{1i, i}, etc., are a set of hp covariant vectors. When the indiccs $i_1 \cdot \cdot i_n$ can be omitted this may be written

$$\mathbf{A} = \sum_{\substack{j=1\\j=1}}^{j=h} \mathbf{a}_{1j} \mathbf{a}_{2j} \cdot \cdot \mathbf{a}_{pj}. \tag{2a}$$

The right member is now identical in appearance with a Gibbs

F. L. Hitchcock, *The Expression of a Tensor or* a Polyadic as a Sum of Products, Journal of Mathematics and Physics, 1927

2. Polyadic form of a tensor.

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$$\mathbf{A} = \sum_{j=1}^{j=h} \mathbf{a}_{1j} \mathbf{a}_{2j} \cdot \cdot \mathbf{a}_{pj}. \tag{2a}$$





 (1_{a})

CP Independently Reinvented (twice) in 1970

CANDECOMP: <u>Can</u>onical <u>Decomp</u>osition

PSYCHOMETRIKA-VOL. 35, NO. 3 BEPTEMBER, 1970

ANALYSIS OF INDIVIDUAL DIFFERENCES IN MULTIDIMEN-SIONAL SCALING VIA AN N-WAY GENERALIZATION OF "ECKART-YOUNG" DECOMPOSITION

J. DOUGLAS CARROLL AND JIH-JIE CHANG

BELL TELEPHONE LABORATORIES MURRAY HILL, NEW JERSEY

An individual differences model for multidimensional scaling is outlined in which individuals are assumed differentially to weight the several dimensions of a common "psychological space". A corresponding method of analyzing similarities data is proposed, involving a generalization of "Eckart-Young analysis" to decomposition of three-way (or higher-way) tables. In the present case this decomposition is applied to a derived threeway table of scalar products between stimuli for individuals. This analysis yields a stimulus by dimensions coordinate matrix and a subject by dimensions matrix of weights. This method is illustrated with data on auditory stimuli and on perception of nations.

There has been an interest for some time in the question of dealing with individual differences among subjects in making similarity judgments on which a multidimensional scaling of stimuli is to be based. Kruskal [1968] and McGee [1968] have both incorporated different ways of dealing with individual differences into their scaling procedures. Tucker and Messick [1963] proposed an approach, which they called "Points of view analysis," which is probably the most widely used method for dealing with such individual differences. In this method, intercorrelations are first computed between subjects (based on their similarity judgments) and the resulting correlation matrix is factor analyzed to produce a subject space. One then looks for clusters of subjects in this subject space, and if such clusters are found, proceeds in one way or another to define "idealized" subjects corresponding to clusters. (The "idealized subject" for a given cluster may be defined, for example, by finding the pattern of similarity judgments corresponding to a hypothetical subject at the cluster centroid, by choosing the actual subject closest to that centroid, or, most simply, by averaging the similarity judgments for subjects in the given cluster.) The similarities for these "idealized subjects" are then, individually and independently, subjected to multidimensional scaling.

This approach has been criticized by a number of people, most recently by Ross [1966] (see Cliff, 1968, for a reply to Ross's criticism and a further discussion of the "idealized individuals" interpretation of "Points of view

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CP: CANDECOMP/PARAFAC

In 2000, Henk Kiers proposed this compromise name

Richard A. Harshman

Univ. Ontario

(1943 - 2008)



2010: Pierre Comon, Lieven DeLathauwer, and others reverse-engineered CP, revising some of Hitchcock's terminology

PARAFAC: <u>Para</u>llel <u>Fac</u>tors

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NOTE: This manuscript was originally published in 1970 and is reproduced here to make it more accessible to interested scholars. The original reference is Harshman, R. A. (1970). Foundations of the PARAFAC procedure: Models and conditions for an "explanatory" multimodal factor analysis. UCLA Working Papers in Phonetics, 16, 1-84. (University Microfilms, Ann Arbor, Michigan, No. 10,085).

FOUNDATIONS OF THE PARAFAC PROCEDURE: MODELS AND CONDITIONS

FOR AN "EXPLANATORY" MULTIMODAL FACTOR ANALYSIS

by Richard A. Harshman U C L A Working Papers in Phonetics 16 December, 1970

Many thanks to the following persons for helping me learn about Jih-Jie Chang: Fan Chung, Ron Graham, Shen Lin (husband), May Chang (niece), Lili Bruer (daughter).

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 (<u>http://frostt.io/tensors/reddit-2015/</u>)
 - 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

For perspective, chance of being struck by lightening in your life ≈ 1 in 10^6

4.7 billion non-zeros (>1 in 10⁹) 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

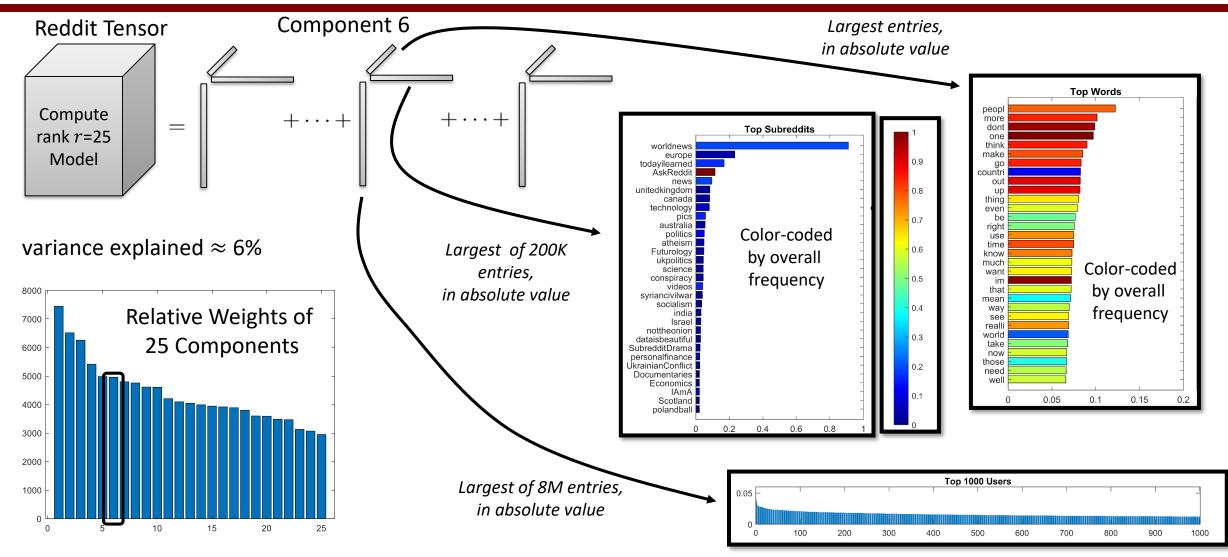
Smith et al (2017). "FROSTT: The Formidable Open Repository of Sparse Tensors and Tools"





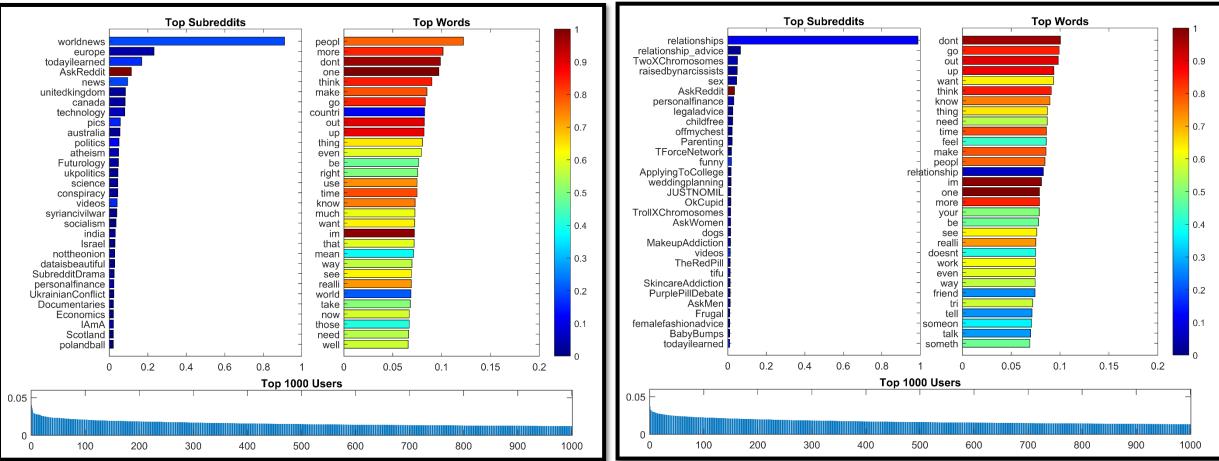


Interpreting Reddit Components





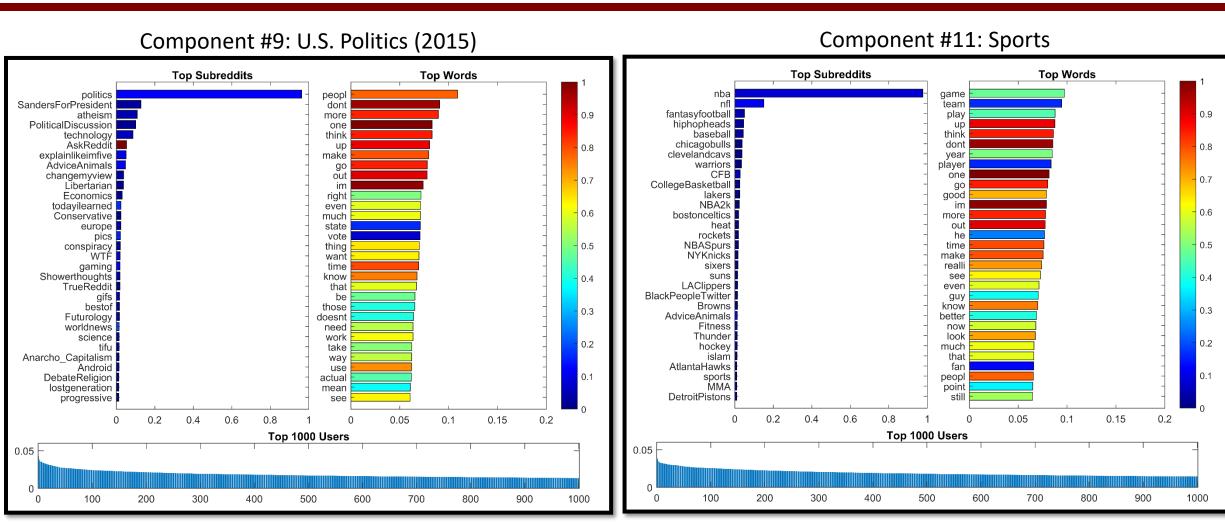




Component #6: International News

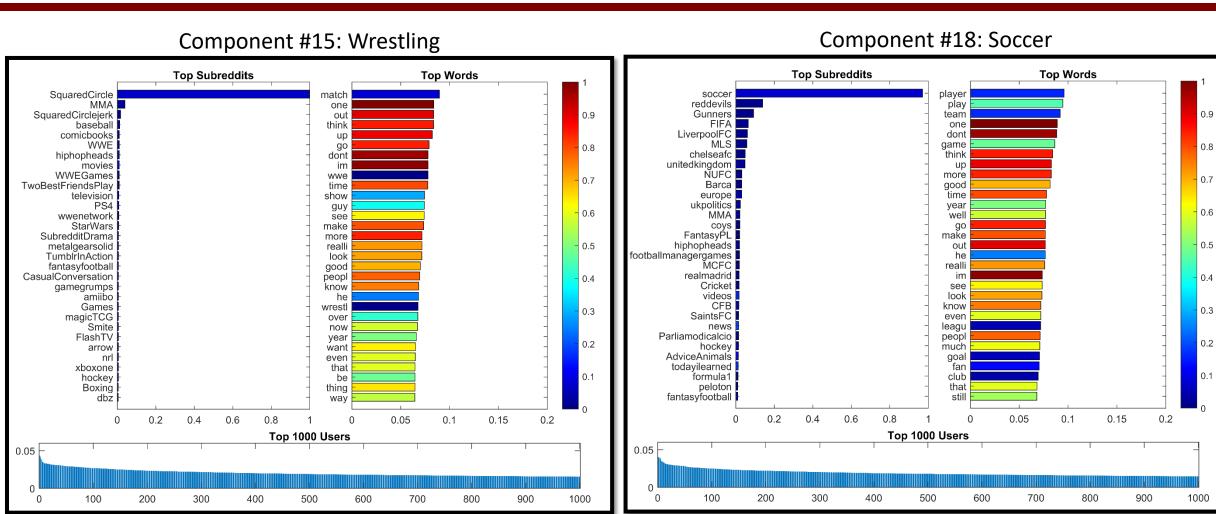
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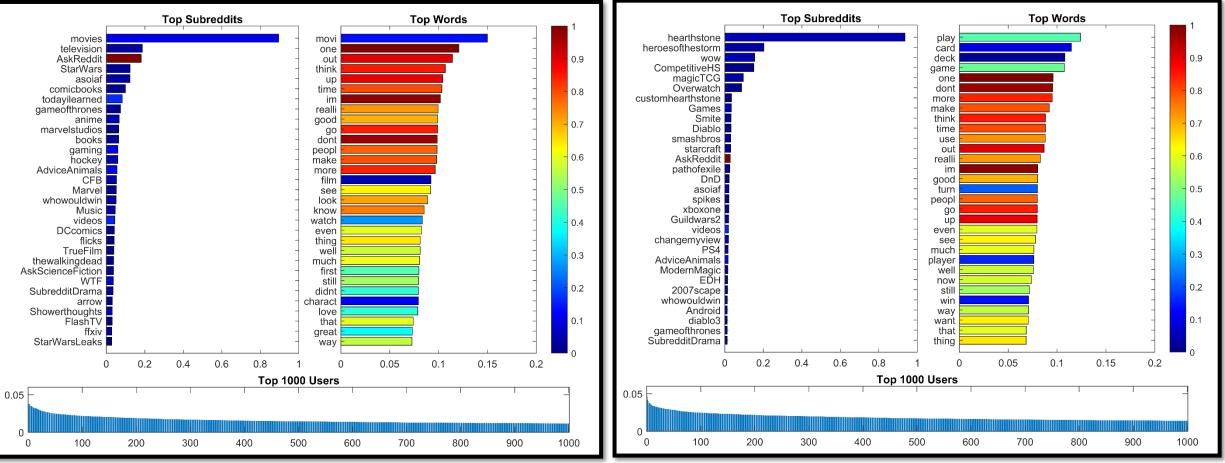




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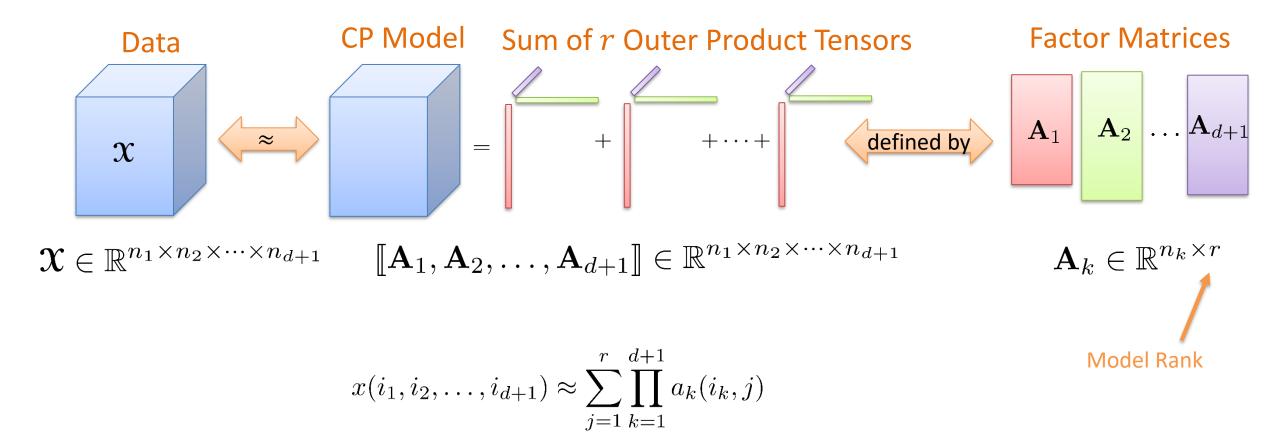
Component #19: Movies & TV

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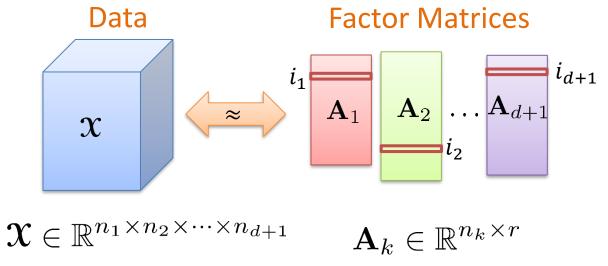




Interpretation as Sum of Outer Products



Interpretation as Row-wise Products



Number of tensor elements = $\prod_{k=1}^{d+1} n_k$

r d+1 $x(i_1, i_2, \dots, i_{d+1}) \approx \sum \prod a_k(i_k, j)$ i=1 k=1

To estimate element $(i_1, i_2, ..., i_{d+1})$ of data tensor

- Extract row i_1 of \mathbf{A}_1
- Extract row i₂ of A₂
- •
- Extract row i_{d+1} of \mathbf{A}_{d+1}
- Multiply extracted rows elementwise
- Sum result 🗉

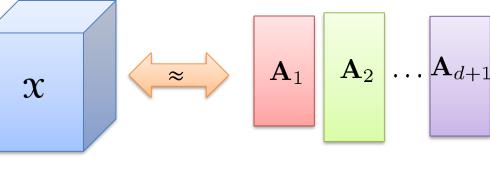
Doing this for every possible combination of rows yields estimates for every element of the data tensor

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Alternating Optimization



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

Data

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

Factor Matrices

$$\min \sum_{i_1=1}^{n_1} \cdots \sum_{i_{d+1}=1}^{n_{d+1}} \left(x(i_1, \dots, i_{d+1}) - \sum_{j=1}^r \prod_{k=1}^{d+1} a_k(i_k, j) \right)^2$$

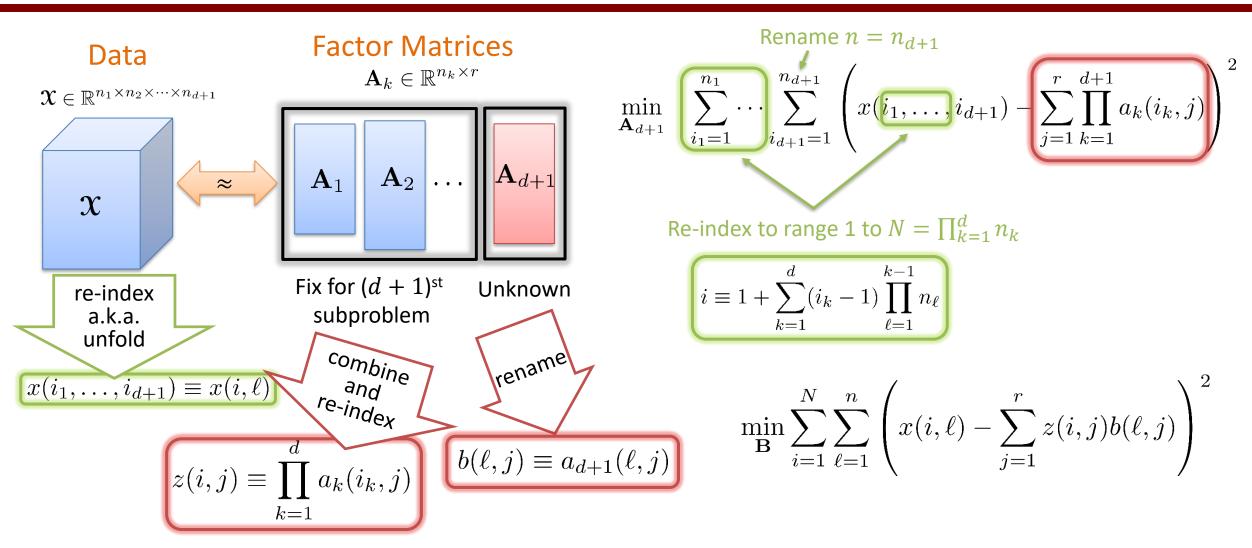
- One approach: Alternating Optimization
- Fix all but one factor matrix and solve for the remaining one
 - Solve for A_1 , fixing A_2 through A_{d+1}
 - Solve for A_2 , fixing A_1 and A_3 through A_{d+1}

- Solve for A_{d+1} , fixing A_1 through A_d
- Repeat until convergence



Alternating Optimization Subproblem is Matrix Linear Least Squares Problem



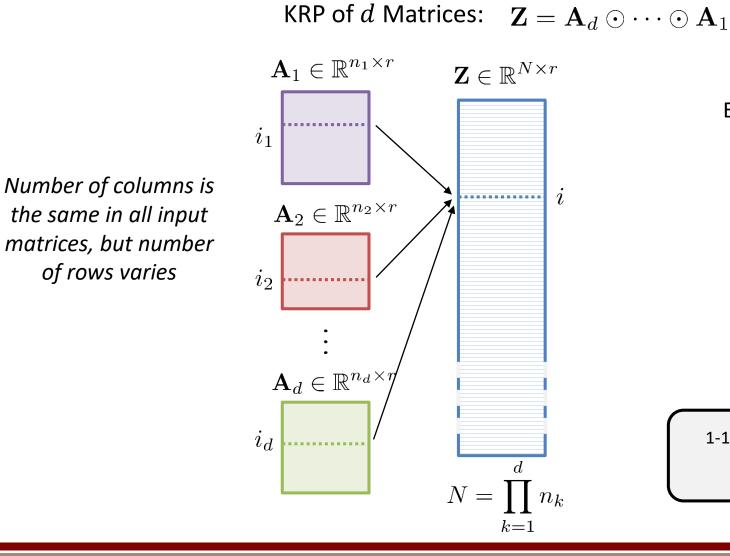


Prototypical CP Least Squares Subproblem is "Tall and Skinny"



$$\min_{\mathbf{B}} \sum_{i=1}^{N} \sum_{\ell=1}^{n} \left(x(i,\ell) - \sum_{j=1}^{r} z(i,j)b(\ell,j) \right)^{2} \qquad \sum_{i=1}^{n} \sum_{\ell=1}^{n} \left(x(i,\ell) - \sum_{j=1}^{r} z(i,j)b(\ell,j) \right)^{2} \qquad \mathbf{Z} \in \mathbb{R}^{N \times r} \quad \mathbf{B}^{\mathsf{T}} \in \mathbb{R}^{r \times n} \qquad \mathbf{X}^{\mathsf{T}} \in \mathbb{R}^{N \times n} \qquad \mathbf{B} = \mathbf{A}_{d+1} \qquad \mathbf{C} = \mathbf{A}_{d} \odot \cdots \odot \mathbf{A}_{1} \qquad \mathbf{X} = \mathbf{X}_{(d+1)} \qquad \mathbf{M} = \mathbf{M}_{d} = \mathbf{M$$

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



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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

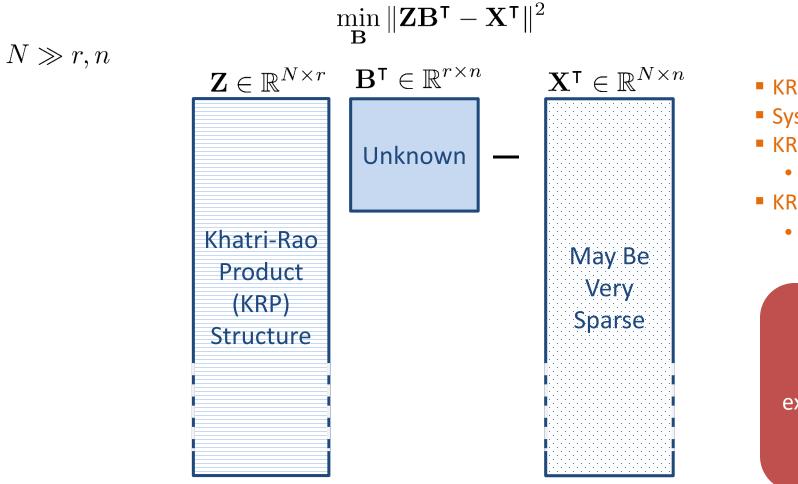
$$i \equiv 1 + \sum_{k=1}^{d} (i_k - 1) \prod_{\ell=1}^{k-1} n_\ell$$

1-1 Correspondence between *linear index and multi index:* $i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \dots \otimes [n_d]$

Prototypical CP Least Squares Problem has Khatri-Rao Product (KRP) Structure





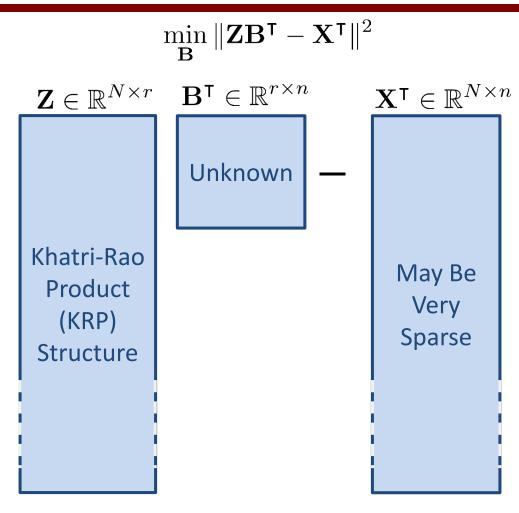


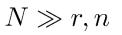
- KRP costs O(Nr) to form
- System costs O(Nnr²) to solve
- KRP structure
 - Cost reduced to O(Nnr)
- KRP structure + data sparse
 - Cost reduced to $O(r \operatorname{nnz}(\mathbf{X}))$

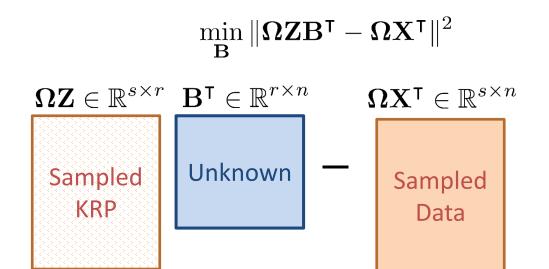
Question for today: Suppose this system is extremely large? How can we solve efficiently?

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









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



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

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

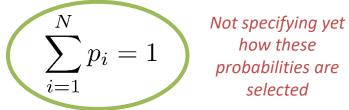
Ingredient #2: Weight Sampled Rows by Probability of Selection to Eliminate Bias

how these

probabilities are

selected

Probability distribution on rows of linear system



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

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

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

$$\begin{split} \mathbb{E} \| \mathbf{\Omega} \mathbf{Z} \mathbf{B}^{\mathsf{T}} - \mathbf{\Omega} \mathbf{X}^{\mathsf{T}} \|^2 &= \sum_{i=1}^{N} p_i \left(\left\| \frac{1}{\sqrt{p_i}} \mathbf{Z}(i,:) \mathbf{B}^{\mathsf{T}} - \frac{1}{\sqrt{p_i}} \mathbf{X}^{\mathsf{T}}(i,:) \right\|^2 \right) \\ &= \| \mathbf{Z} \mathbf{B}^{\mathsf{T}} - \mathbf{X}^{\mathsf{T}} \|^2 \end{split}$$

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

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

Not specifying vet how s is determined

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

Each row has a single nonzero!

Then, as before, we have:

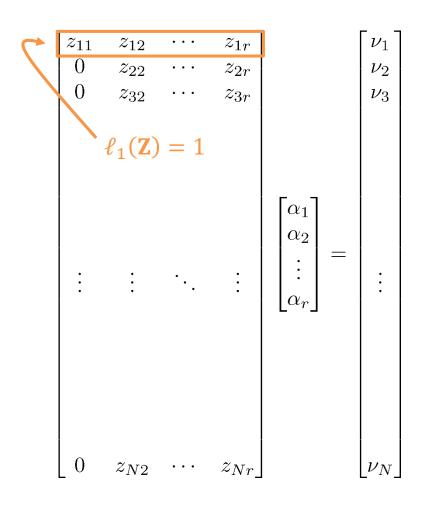
$$\mathbb{E} \| \mathbf{\Omega} \mathbf{Z} \mathbf{B}^{\mathsf{T}} - \mathbf{\Omega} \mathbf{X}^{\mathsf{T}} \|^{2} = \| \mathbf{Z} \mathbf{B}^{\mathsf{T}} - \mathbf{X}^{\mathsf{T}} \|^{2}$$

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

Optimal Choice for Sampling Probability is Based on Leverage Scores







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

What if we do uniform sampling? $p_i = \frac{1}{N}$ 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)

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

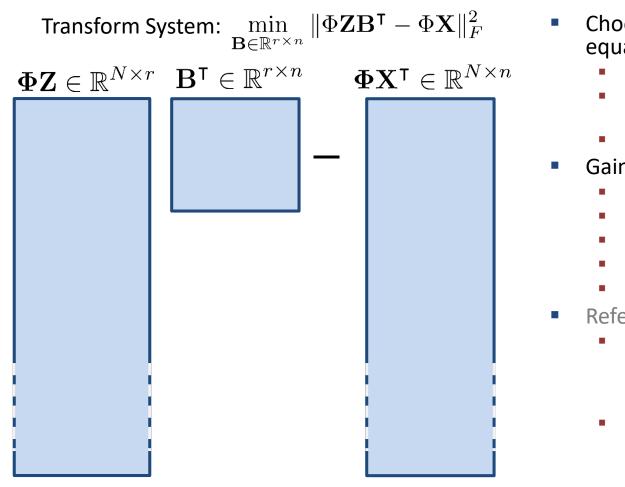
In Case 2, prefer $p_i = \ell_i(\mathbf{Z})/r$, but costs $O(Nr^2)$ to compute leverage scores!

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

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



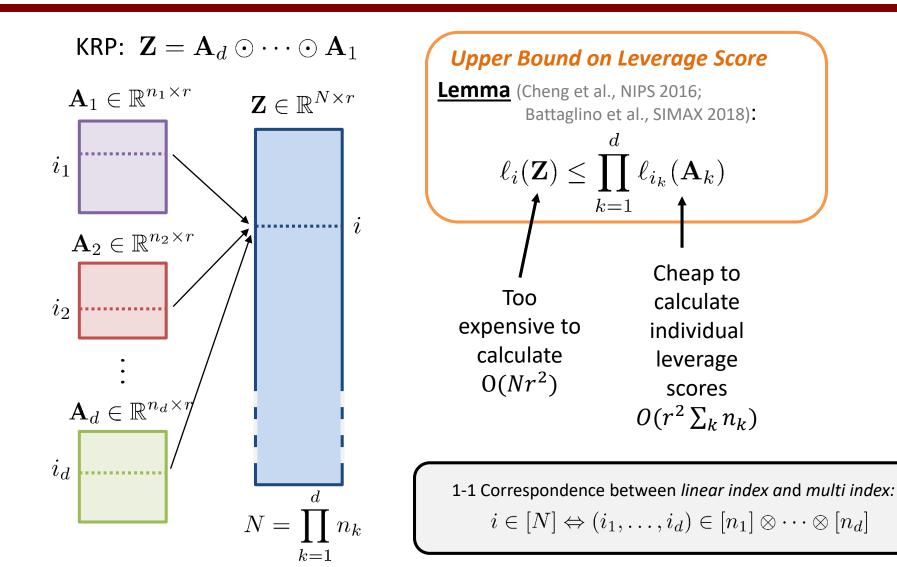




- Choose Φ so that all leverage scores of ΦZ approximately equal, then uniform sampling yields $\beta \approx 1$
 - "Uniformize" the leverage scores per Mahoney
 - Fast Johnson-Lindenstrauss Transform (FJLT) uses random rows of matrix transformed by FFT and Rademacher diagonal
 - FJLT cost per iteration: $O(rN \log N)$
 - 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. <u>https://doi.org/10.1137/17M1112303</u>
 - R. Jin, T. G. Kolda, R. Ward. Faster Johnson-Lindenstrauss Transforms via Kronecker Products, 2019. <u>http://arxiv.org/abs/1909.04801</u>



Ingredient #3: Bound Leverage Scores



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





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

Define sampling probabilities:

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

And random Pick a *s* random indices ξ_j such that sampling matrix: $P(\xi_i = i) = p_i$ and define

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

Solve sampled problem:

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

Get probabilistic error bound:

With probability $1 - \delta$ for $\delta \in (0,1)$, we have $\|\mathbf{Z}\tilde{\mathbf{B}}_*^{\mathsf{T}} - \mathbf{X}^{\mathsf{T}}\|$

$$\|\mathbf{Z}\tilde{\mathbf{B}}_*^{\mathsf{T}} - \mathbf{X}^{\mathsf{T}}\|_F^2 \le (1 + O(\epsilon))\|\mathbf{Z}\mathbf{B}_*^{\mathsf{T}} - \mathbf{X}^{\mathsf{T}}\|_F^2$$

when number of samples satisfies:

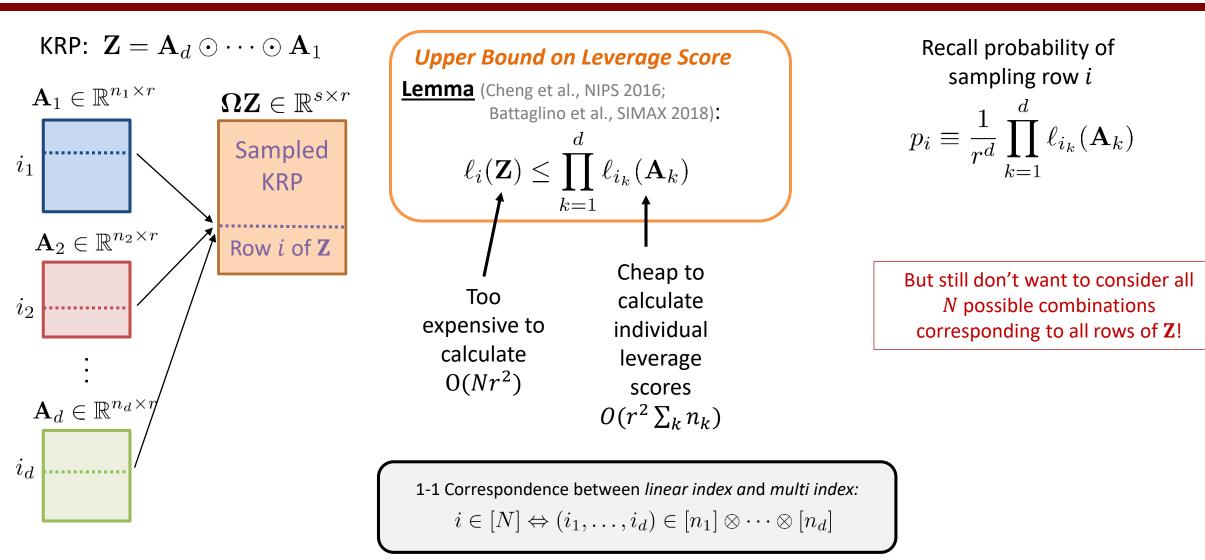
$$s = O(r^d \log(n/\delta)/\epsilon^2)$$

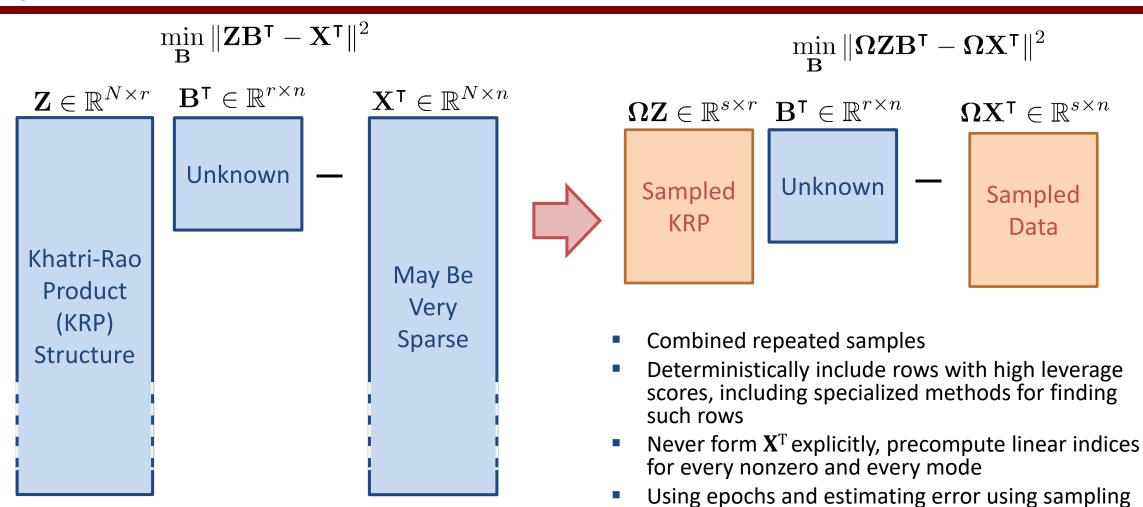
1-1 Correspondence between *linear index and multi index:* $i \in [N] \Leftrightarrow (i_1, \dots, i_d) \in [n_1] \otimes \dots \otimes [n_d]$

Ingredient #5: Efficient Sampling <u>without</u> Forming KRP









See Reference for Details of Other Specializations

10/6/2020

Kolda - Sayas Seminar

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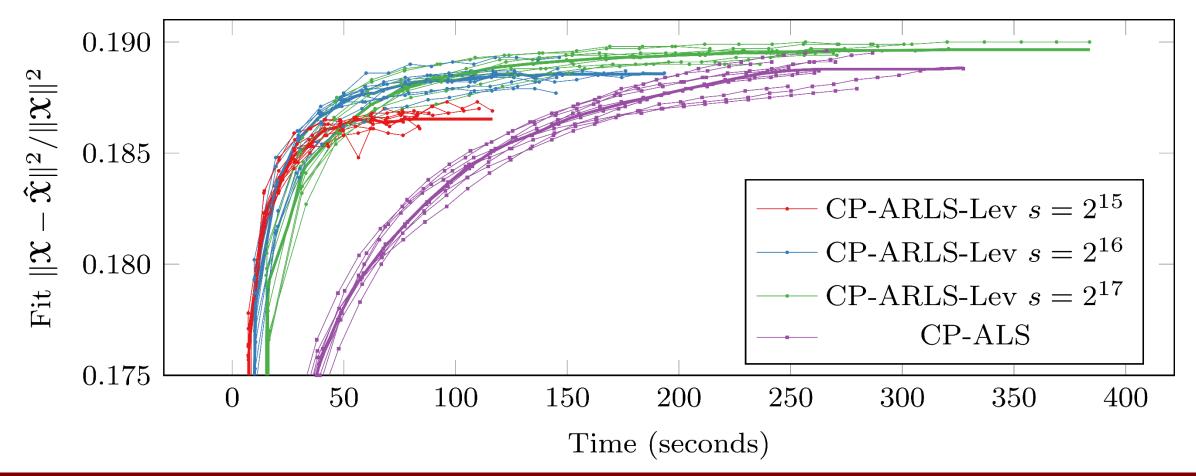
Numerical Results

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CP-ARLS-Lev Comparable to CP-ALS on Small Uber Problem



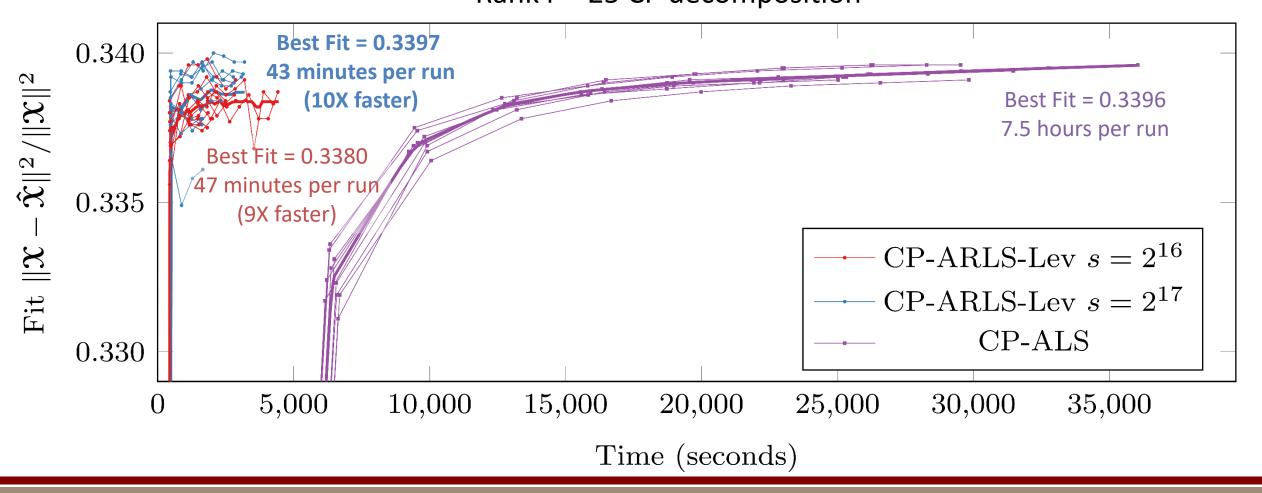
Uber Tensor: 183 x 24 x 1140 x 1717 Uber Tensor with 3M nonzeros (0.038% dense). Rank r = 25 CP decomposition



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



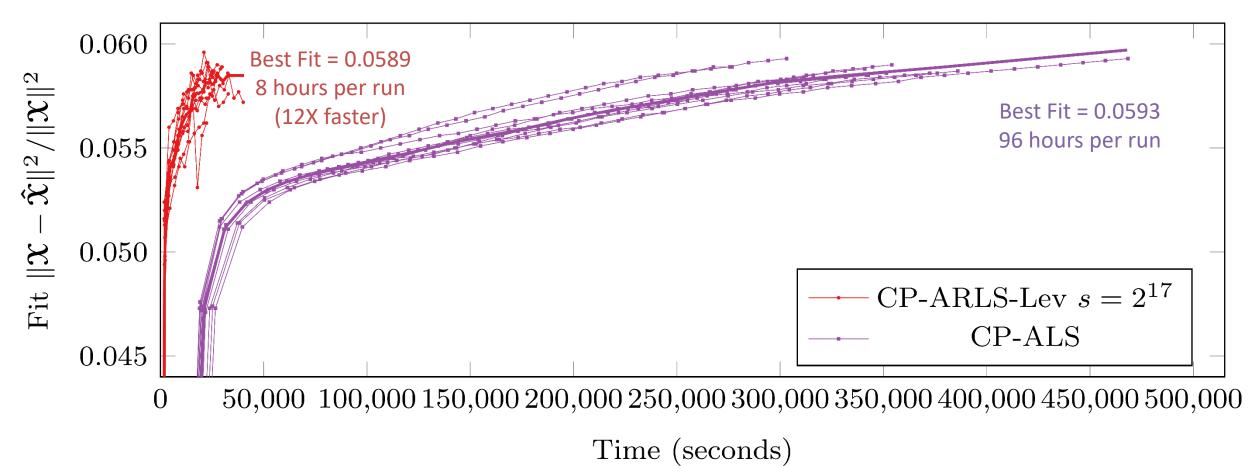
Amazon Tensor: 4.8M x 1.8M x 1.8M Amazon Tensor with 1.7B nonzeros. Rank r = 25 CP decomposition

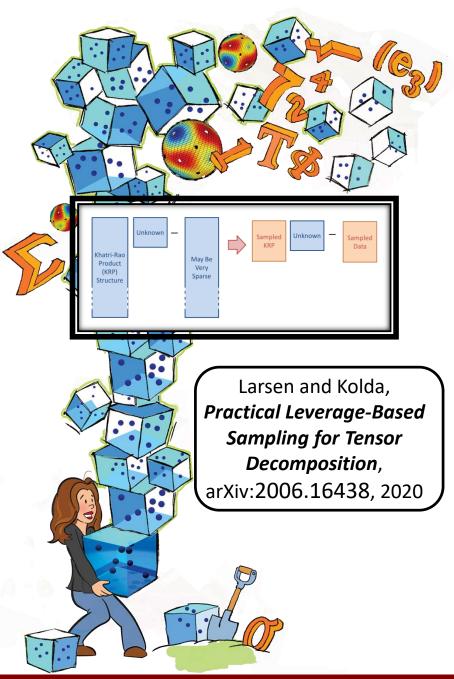


Over 12X Speed-up for Reddit Tensor with 4.7 Billion Nonzeros (106 GB)



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







ries

Conclusions & Future Work

- Tensor decomposition: unsupervised machine learning
- Many applications, including social discussion analysis
- Model fit via alternating optimization, resulting in series of least squares subproblems
- Subproblems are "tall and skinny", amenable to sketching
- Leverage-score sampling ideal for sparse data tensors
- Can estimate leverage scores cheaply using leverage scores of factor matrices
- Results in huge speedups f

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