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Fast Exact Leverage Score Sampling from Khatri-Rao Products with Applications to Tensor Decomposition

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NEURAL INFORMATION PROCESSING SYSTEMS

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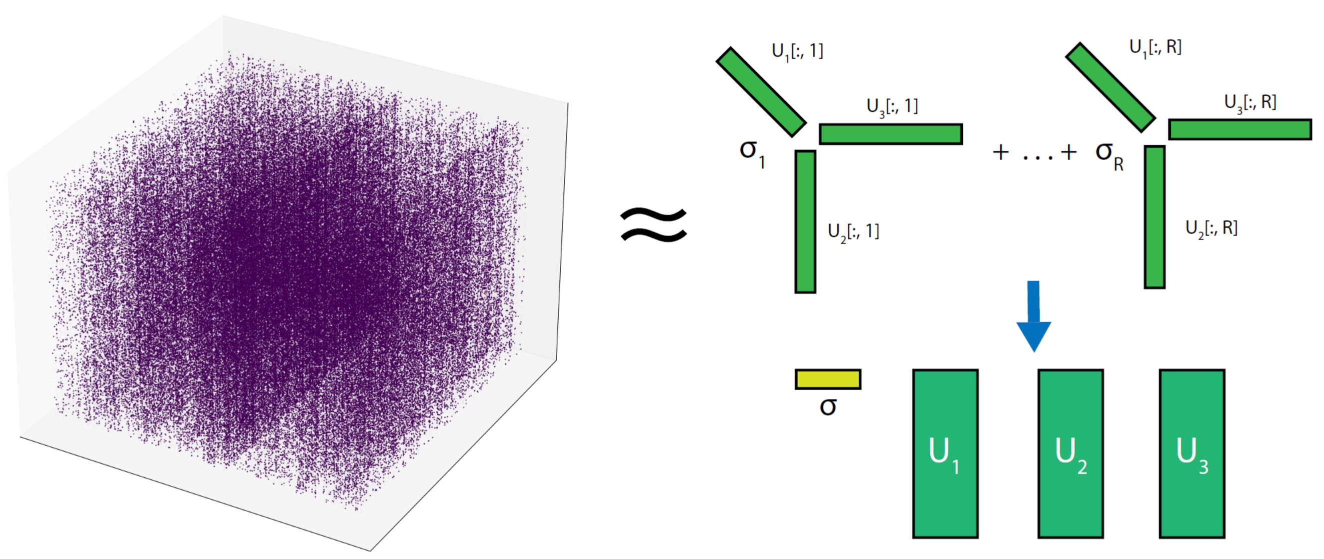
Sparse Tensor Decomposition and Khatri-Rao Products

Motivating Application: Given an $(N+1)$-dimensional sparse tensor $\mathcal{T}$, compute an approximate Candecomp / PARAFAC decomposition:



Decomposition of rank R consists of factor matrices $U_j \in \mathbb{R}^{I_j \times R}$, $1 \leq j \leq N+1$ to store the outer product components, vector $\sigma \in \mathbb{R}^R$ to store generalized singular values. Want to capture values of nonzero entries AND locations of zero entries. Problem is non-convex and NP-hard.

Alternating Least-Squares (ALS): Iteratively optimize one factor at a time while keeping the others constant (also called block coordinate descent). Optimization problem for U_{N+1} is an overdetermined linear least-squares problem

$$\min_X \|AX - B\|_F \qquad (1)$$

where $A = U_N \odot \ldots \odot U_1$, B is a sparse matrix. $\odot$ denotes a Khatri-Rao Product (KRP), a column-wise Kronecker Product of two matrices:

$$\begin{bmatrix} a & b \\ c & d \end{bmatrix} \odot \begin{bmatrix} w & x \\ y & z \end{bmatrix} = \begin{bmatrix} aw & bx \\ cw & dx \\ ay & bz \\ cy & dz \end{bmatrix}$$

Least-squares problems of this form also arise in PDE-inverse problems, signal processing, and compressed sensing.

Leverage Score Sampling

Problem: Design matrix A from Equation (1) has $\prod_{j=1}^N I_j$ rows. May not even fit in memory!

Solution: Generate random sampling matrix S with $J \ll \prod_{j=1}^N I_j$ rows, solve

$$\min_{\tilde{X}} \|SA\tilde{X} - SB\|_F.$$

Choosing S as a sampling matrix preserves sparsity of B. To guarantee residual within $(1+\varepsilon)$ of true minimum w.h.p. $(1-\delta)$, sample $\tilde{O}(R/(\varepsilon\delta))$ rows proportional to leverage scores:

$$\ell_i = A[i,:](A^\top A)^+ A[i,:]^\top$$

Central Challenge: How do we sample rows according to the leverage score distribution of A when even materializing A is too expensive?

Our Contributions

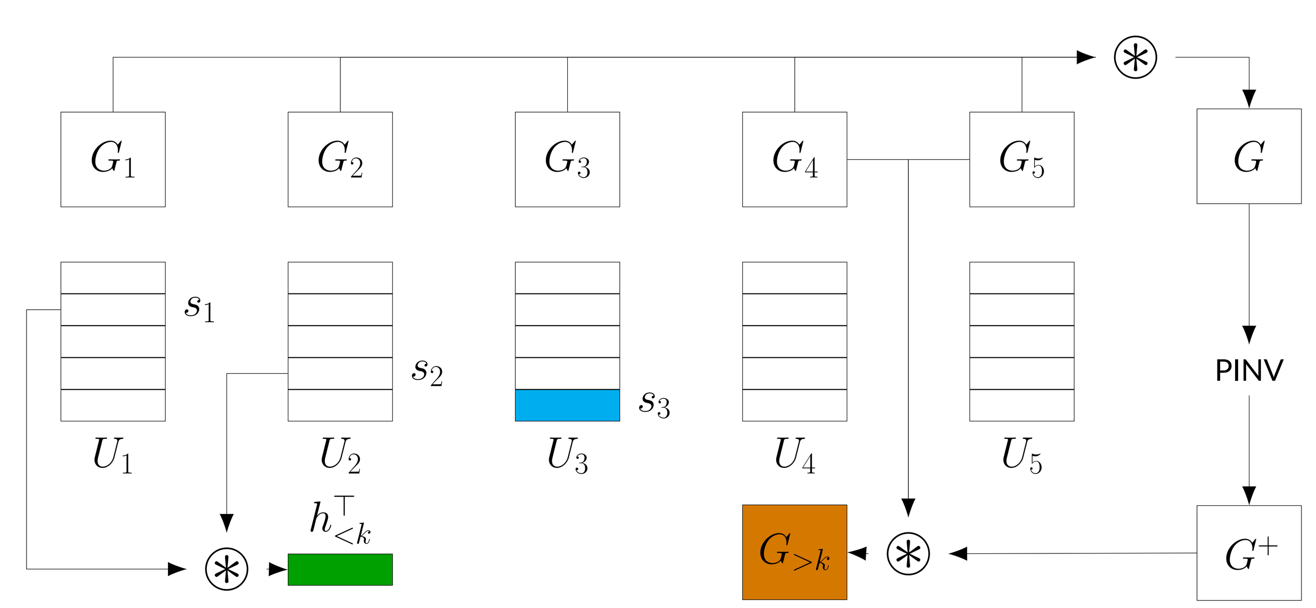
We build a data structure to sample rows from the exponentially tall matrix A in time logarithmic in its row count and quadratic in its column count from the exact leverage score distribution. To decompose an $(N+1)$-dimensional tensor, our method achieves the lowest asymptotic runtime for sketched CP decomposition compared to recent SOTA methods.

Method	Complexity per ALS Round
CP-ALS [1]	$N(N+I)I^N R$
CP-ARLS-LEV [2]	$N(R+I)R^{N+1}/(\varepsilon\delta)$
TNS-CP [3]	$N^3 I R^3/(\varepsilon\delta)$
GTNE [4]	$N^2(N^{1.5}R^{3.5}/\varepsilon^3 + IR^2)/\varepsilon^2$
STS-CP (ours)	$N(NR^3 \log I + IR^2)/(\varepsilon\delta)$

Our method accelerates decomposition of sparse tensors with billions of nonzero entries.

Methodology

Sample rows from $U_1, \ldots, U_N$ in sequence, each conditioned on the last.

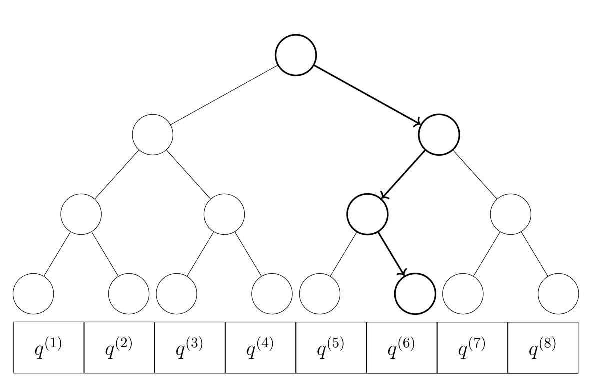


Conditional Distribution: $q[s_k] = p(\hat{s}_k = s_k \mid \hat{s}_{<k} = s_{<k}) \propto \langle h_{<k} h_{<k}^\top, U_k[s_k,:]^\top U_k[s_k,:], G_{>k} \rangle$

Sampling Procedure: Sample $r \sim \mathrm{Unif}[0,1]$, find "containing bin" of width q_j via **binary search.**

Root: branch right iff $\sum_{j=0}^{I_k/2} q[j] < r$

Level 2: branch right iff $\sum_{j=0}^{I_k/2} q[j] + \sum_{j=I_k/2}^{3I_k/4} q[j] < r$...



Key: For nodes v in search tree corresponding to row interval $[S_0(v), S_1(v)]$ (up to level $\log(I_k/R)$), compute and store "partial gram matrix":

$$G^v = \sum_{i=S_0(v)}^{S_1(v)} U_k[i,:]^\top U_k[i,:]$$

Construction runtime is $O(I_k R^2)$ with storage requirement $O(I_k R)$. During sampling, computing the branch decision at each internal node costs $O(R^2)$ with cached partial gram matrices. $O(R^3)$ work required below level $\log(I_k/R)$, but can improve to $O(R^2 \log R)$ (see paper). Total time per sample is $O(R^2 \log I_k)$.

Runtime Benchmarks

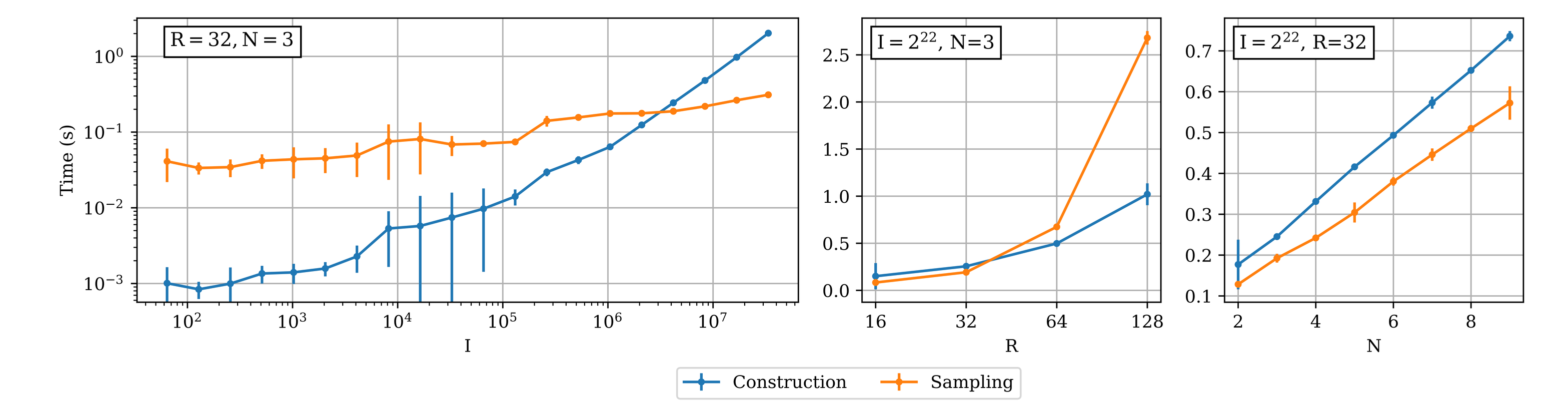


Figure 1. Average Time to Construct Data Structure and Draw 50,000 Samples from Khatri-Rao Product.

Sparse Tensor Experiments

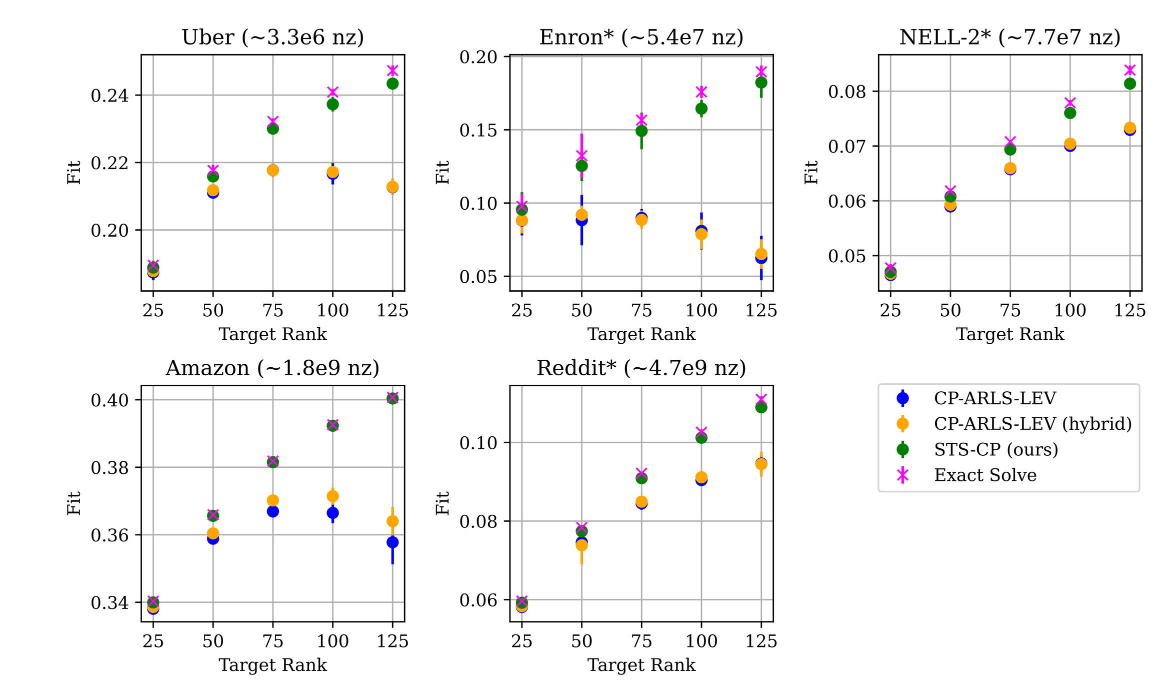


Figure 2. Accuracy Achieved by CP-ARLS-LEV, STS-CP, and Exact ALS on Sparse Tensor Decomposition, $J = 2^{16}$ samples for randomized algorithms.

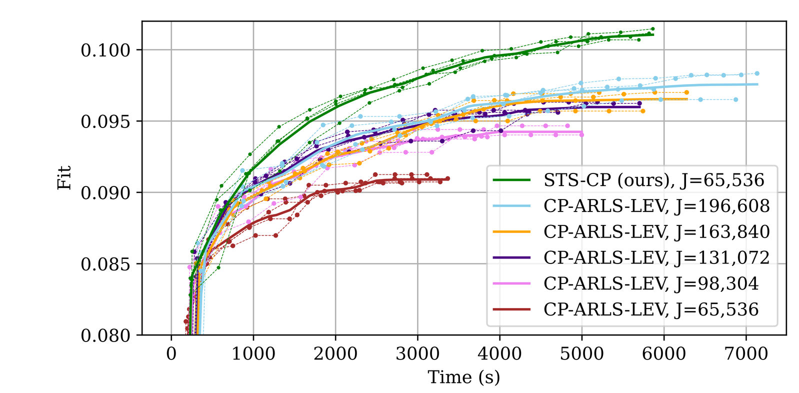


Figure 3. Fit vs. Time, Reddit Tensor (4.8 billion nonzeros) for CP-ARLS-LEV and STS-CP (ours). Thick lines are averages of individual traces.

Acknowledgements and References

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