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Leverage-Based Sketches for Khatri-Rao Products

Redwood Center for Theoretical Neuroscience

November 1, 2024

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The Berkeley BeBOP and PASSION Groups

I work with two groups at UC Berkeley:

- The **B**erkeley **Be**nchmarking and **Op**timization (BeBOP) group led by James Demmel and Katherine Yelick.
- The **P**arallel **A**lgorithms for **S**calable **S**parse computatIONs (PASSION) group led by Aydın Buluç, joint with Lawrence Berkeley National Lab.

Our interests include **linear algebraic computations** and **sparse kernels** that can be parallelized and deployed at **supercomputer scale**.

Figure: Frontier, the first exascale supercomputer in the United States. Credit: OLCF, Wikimedia Commons CC2.0.

Link to Today's Paper

Fast Exact Leverage Score Sampling From Khatri-Rao Products with Applications to Tensor Decomposition [Bha+23]. Link to paper below, more at `https://vivek-bharadwaj.com`.

Introduction

The Khatri-Rao Product

- In this talk, the Khatri-Rao product (KRP, denoted $\odot$) is the column-wise Kronecker product of two matrices:

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

- Output column count is *identical* to inputs. Output row count is the *product* of row counts of inputs.

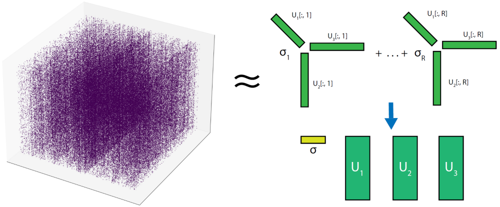
- Appears in signal processing, compressed sensing, PDE inverse problems. Possible use in hyperdimensional computing where $\otimes$, the Kronecker product, used for binding.

Motivating Application

- **Our goal:** efficiently solve an overdetermined linear least-squares problem

$$\min_X \|AX - B\|_F$$

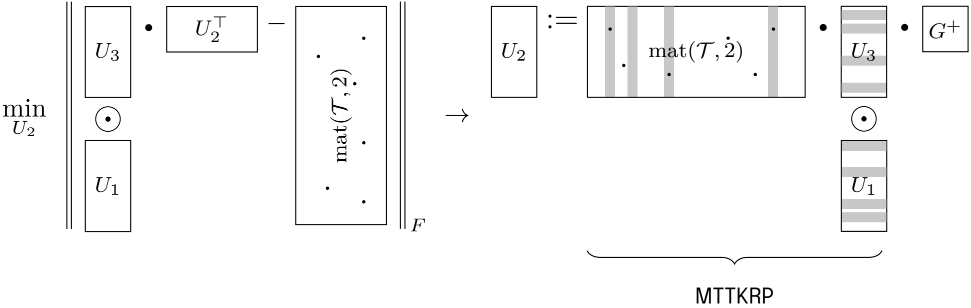
where $A = U_1 \odot \ldots \odot U_N$ with $U_j \in \mathbb{R}^{I \times R}$.



- Key kernel in alternating least-squares Candecomp / PARAFAC (CP) decomposition [LK22].

One Step of ALS Illustrated

$$\min_{U_j} \left\| \left[\bigodot_{k\neq j} U_k \right] \cdot U_j^\top - \mathrm{mat}(\mathcal{T}, j)^\top \right\|_F$$



Randomized Linear Least-Squares

- **Sketch & Solve**: Apply short-wide sketching matrix S to both A and B, solve reduced problem
$$\min_{\tilde{X}} \left\| SA\tilde{X} - SB \right\|_F$$
- Want an (ε, δ) guarantee on solution quality: with high probability $(1-\delta)$,
$$\left\| A\tilde{X} - B \right\|_F \leq (1+\varepsilon) \min_X \|AX - B\|$$
- Could choose S as:
  - An i.i.d. Gaussian / Rademacher random matrix
  - A Countsketch / Sparse Sign embedding (fixed nnz per column)
  - A composition of random diagonal, FFT-like operator, and uniform sparse sampler

Subspace Embedding Matrices

i.i.d. Gaussian

$$\begin{bmatrix} -0.01 & -0.39 & 0.37 \\ -0.47 & 0.74 & -0.10 \end{bmatrix}$$

Countsketch

$$\begin{bmatrix} +1 & 0 & +1 \\ 0 & -1 & 0 \end{bmatrix}$$

- Oblivious subspace embeddings: require no prior information about A; easy to construct and apply when inputs have no structure, but harder for Khatri-Rao products.
- In this talk: we will just **randomly sample** J rows of A and B to form a pair of much shorter matrices. Preserves structure in both input and output.

Our Contributions [Bha+23]

Method	Source	Round Complexity ($\tilde{O}$ notation)
CP-ALS	[KB09]	$N(N+I)I^{N-1}R$
CP-ARLS-LEV	[LK22]	$N(R+I)R^N/(\varepsilon\delta)$
TNS-CP	[Mal22]	$N^3IR^3/(\varepsilon\delta)$
GTNE	[MS22]	$N^2(N^{1.5}R^{3.5}/\varepsilon^3 + IR^2)/\varepsilon^2$
STS-CP	Ours	$N(NR^3 \log I + IR^2)/(\varepsilon\delta)$

- We build a data structure with runtime **logarithmic** in the height of the KRP and quadratic in R to sample from *leverage scores* of A.
- Yields the **STS-CP** algorithm: lower asymptotic runtime for randomized dense CP decomposition than recent SOTA methods (even more advantage for sparse tensors).

Statistical Leverage Scores

Intuition: Do I Need Every Row?

- Consider a univariate regression problem with 100,000 (x, y) points.
- This is a **highly-overdetermined** problem. Can pick a subset of points to perform fitting.

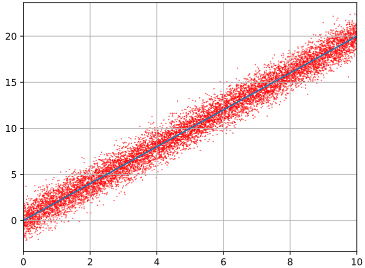


Figure: $y_i \sim x_i + \mathcal{N}(0, 1)$

Leverage Score Sampling

We will sample rows i.i.d. from A according to the *leverage score distribution* on its rows. Given **reduced SVD** $A = U\Sigma V^\top$, the leverage score ℓ_i of row i is

$$\ell_i = \|U[i,:]\|^2 .$$

Theorem (Leverage Score Sampling Guarantees, [Mal22])

Suppose $S \in \mathbb{R}^{J\times I}$ is a leverage-score sampling matrix for $A \in \mathbb{R}^{I\times R}$, and define

$$\tilde{X} := \arg\min_{\tilde{X}} \left\|SA\tilde{X} - SB\right\|_F$$

If $J \gtrsim R\max(\log(R/\delta), 1/(\varepsilon\delta))$, then with probability at least $1-\delta$,

$$\left\|A\tilde{X} - B\right\|_F \leq (1+\varepsilon)\min_X \|AX - B\|_F .$$

Interpretation of Leverage Scores

When A has 1 column, leverage scores are proportional to squared distance from origin.

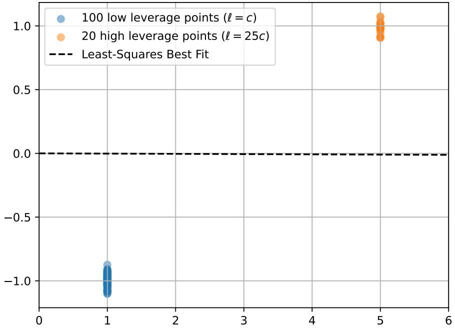
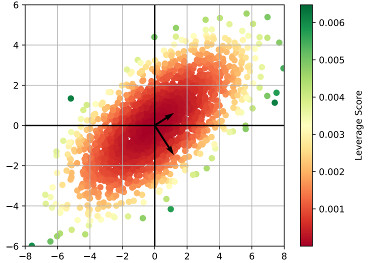


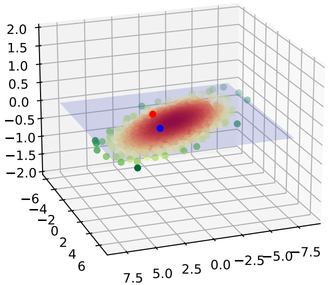
Figure: A univariate regression problem with low and high leverage points (intercept constrained to be 0).

Interpretation of Leverage Scores

In general, leverage scores of A quantify *influence* that each row has on the solution, capture correlation of rows of A with rows of $\Sigma^{-1}V^\top$.



(a) Projection onto xy-plane



(b) (x, y, z) data

Figure: Leverage scores of $(x, y, 0)$ triples from a multivariate normal distribution. Left: components of $\Sigma^{-1}V^\top$ shown. Right: the red point has greater influence than the blue point (both equidistant from $(0, 0, 0)$).

Interpretation of Leverage Scores

- Leverage score sampling captures the geometry of the column space of A.
- Rigorously: sampling i.i.d. with leverage score probabilities leads to an **optimal** [DM20] sample complexity to construct an ℓ_2-subspace embedding matrix S.
- **SE Property:** W.h.p simultaneously for ALL vectors $x \in \mathbb{R}^R$,

$$(1-\tilde{\varepsilon})\,\|Ax\|_2 \leq \|SAx\|_2 \leq (1+\tilde{\varepsilon})\,\|Ax\|_2$$

- In turn, an ℓ_2-S.E. guarantees that our sketched solution has close-to-optimal residual with respect to the original problem.

Prior Work

Problem: Cost to compute all leverage scores exactly is identical to runtime of QR decomposition. Defeats the purpose of sampling!

- (SPALS [Che+16]): Sample rows according to *approximate* leverage scores of A. Worst-case **exponential** in N to achieve (ε, δ) guarantee.

- (CP-ARLS-LEV [LK22]): Similar approximation, hybrid random-deterministic sampling strategy and practical improvements.

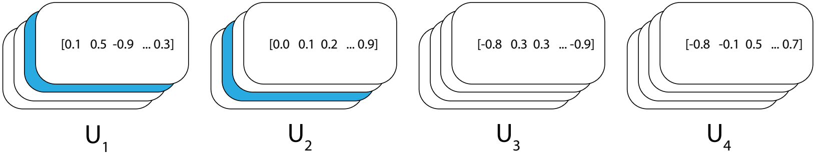
- (TNS-CP [Mal22]): Samples implicitly from exact leverage distribution with **polynomial** complexity to achieve (ε, δ) guarantee, but linear dependence on I for each sample. **We want to accelerate this algorithm.**

Efficient Sampling from Khatri-Rao Products

Implicit Leverage Score Sampling

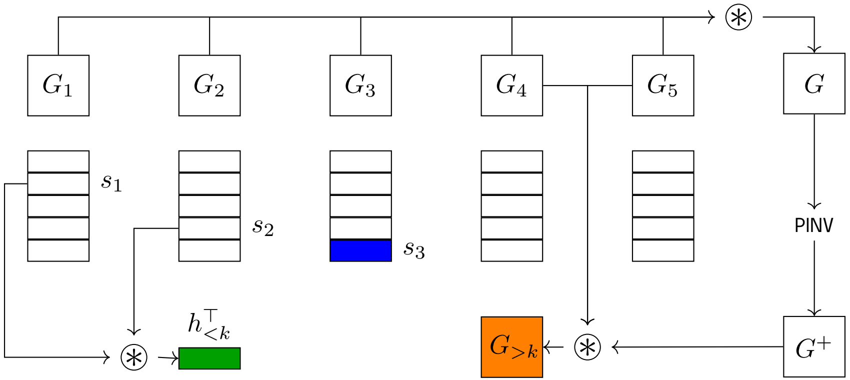
- For $I = 10^7, N = 3$, matrix A has 10^{21} rows. Can't even index rows with 64-bit integers. Instead: use identity $\ell_i = A[i,:]\,(A^\top A)^+ A[i,:]^\top$.

- Draw a row from each of $U_1, ..., U_N$, return their Hadamard product.



- Let $\hat{s}_j$ be a random variable for the row index drawn from U_j. Assume $(\hat{s}_1, ..., \hat{s}_N)$ jointly follows the leverage score distribution on $U_1 \odot ... \odot U_N$.

The Conditional Distribution of $\hat{s}_k$



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

A Problem of Variable Dependence

- Each subsequent index depends on the ones that precede it. How to deal with the dependence? Let's look at four approaches:

- Only a finite number of values for $\hat{s}_1, \hat{s}_2$. Precompute and store all possible conditional distributions for $\hat{s}_3$, and similarly for $\hat{s}_4, \hat{s}_5 \ldots$

- Preprocessing time is $\Omega\left(I^N\right)$, not viable for large I.

Preprocessing Time	Time for J Samples	# Samples Required
$\Omega(I^N)$	$O(JN)$	$O(R/(\varepsilon\delta))$

Approach 2: Ignore the Dependence

- Sample **independently** from $U_1, ..., U_N$ based on the leverage scores of each factor matrix [Che+16; LK22].
- No longer sampling from the exact leverage score distribution, so require $O(R^N/(\varepsilon\delta))$ samples to achieve the (ε, δ) guarantee.
- Efficient if R, N low enough. Can easily update if one matrix U_j changes.

Preprocessing Time	Time for J Samples	# Samples Required
$O(NIR^2)$	$O(JN)$	$O(R^N/(\varepsilon\delta))$

Approach 3: Form Full Conditional Distribution

- Compute the full conditional distribution $p(\hat{s}_3 = s_3 \mid \hat{s}_1 = s_1, \hat{s}_2 = s_2)$ for each draw *during* sampling [Mal22].
- Costs $O(IR^2)$ per matrix U_j **per sample**.
- Works well if I is low enough (many dense tensor applications), but performance degrades for $I \geq 10^3$.

Preprocessing Time	Time for J Samples	# Samples Required
$O(NIR^2)$	$O(JNR^2I)$	$O(R/(\varepsilon\delta))$

Approach 4: Segment Tree Sampling (Ours)

- Our approach will require only $O(NR^2 \log I)$ time per sample, after one-time preprocessing costs of $O(IR^2 + R^3)$ per matrix.
- For $R \approx 10^2$, we achieve a sampling time that is practical for sparse tensor decomposition with mode sizes in the tens of millions.

Preprocessing Time	Time for J Samples	# Samples Required
$O(NIR^2)$	$O(NR^3 + JNR^2 \log I)$	$O(R/(\varepsilon\delta))$

Key Sampling Primitive

$$q[i] := C^{-1} \langle h_{<k} h_{<k}^{\top}, U_k[i,:]^{\top} U_k[i,:], G_{>k} \rangle$$

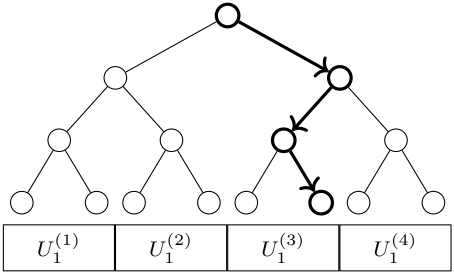
- Imagine we magically had all entries of q - how to sample? Initialize I bins, j-th has width $q[j]$.
- Choose random real r in $[0,1]$, find "containing bin" i such that

$$\sum_{j=0}^{i-1} q[j] < r < \sum_{j=0}^{i} q[j]$$

Binary Tree Inversion Sampling

- Locate bin via binary search (truncated to $\log(I/R)$ levels)
- Root: branch right iff $\sum_{j=0}^{I/2} q\left[j\right] < r$
- Level 2: branch right iff

$$\sum_{j=0}^{I/2} q\left[j\right] + \sum_{j=I/2}^{3I/4} q\left[j\right] < r$$



Key: Can compute summations quickly if we cache information at each node!

Caching Partial Gram Matrices

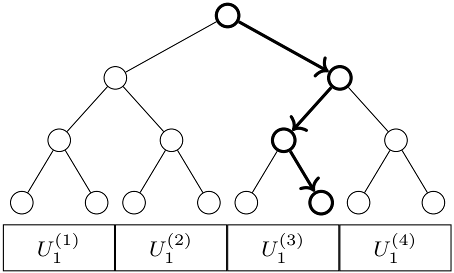
Let an internal node v correspond to an interval of rows $[S(v)...E(v)]$.

$$
\begin{aligned}
\sum_{j=S(v)}^{E(v)} q[j] &= \sum_{j=S(v)}^{E(v)} C^{-1}\langle h_{<k}h_{<k}^\top, U_k[j,:]^\top U_k[j,:], G_{>k}\rangle \\
&= C^{-1}\langle h_{<k}h_{<k}^\top, \sum_{j=S(v)}^{E(v)} U_k[j,:]^\top U_k[j,:], G_{>k}\rangle \\
&= C^{-1}\langle h_{<k}h_{<k}^\top, U_k[S(v):E(v),:]^\top U_k[S(v):E(v),:], G_{>k}\rangle \\
&:= C^{-1}\langle h_{<k}h_{<k}^\top, G^v, G_{>k}\rangle
\end{aligned} \tag{1}
$$

Can compute and store G^v for ALL nodes v in time $O(IR^2)$, storage space $O(IR)$. Use BLAS-3 **syrk** calls in parallel to efficiently construct the tree.

Efficient Sampling after Caching

- At internal nodes, compute $C^{-1}\langle h_{<k} h_{<k}^\top, G^v, G_{>k} \rangle$ in $O(R^2)$ time (read normalization constant from root)
- At leaves, spend $O(R^3)$ time to compute remaining values of q. Can reduce to $O(R^2 \log R)$, see paper.
- Complexity per sample: $O(NR^2 \log I)$ (summed over all tensor modes).



An Empirical Correctness Check

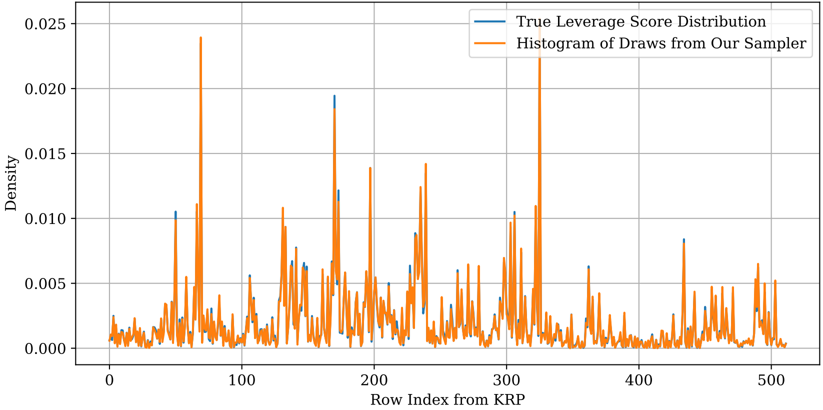


Figure: Distribution Comparison for $U_1 \odot U_2 \odot U_3, U_j \in \mathbb{R}^{8 \times 8}$ initialized i.i.d. Gaussian.

Remarks and Related Work

- The most comparable results to ours appear in work by Woodruff and Zandieh [WZ22], who construct a leverage-score sampler with **input-sparsity runtime**.

- Their sampler can also be used for low-rank approximation, but has $O(N^7)$ worst-case scaling in the KRP dimension.

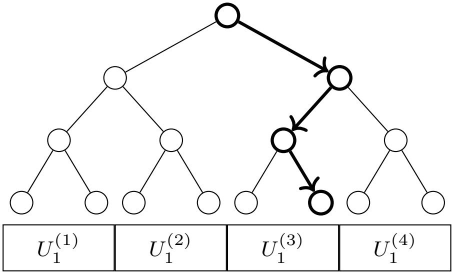
- The best existing **oblivious algorithms** for Khatri-Rao products require either:
  - $\Omega(R^2)$ rows to construct a subspace embedding [Ahl+20].
  - More than input-sparsity runtime.

- **Open Question:** Is LSS **more powerful** than oblivious embedding for Khatri-Rao products, and can we prove a lower bound?

Performance Measurements

High-Performance Parallel Sampling

- We want to execute $J \sim 50,000$ independent random walks down a full, complete tree.
- At each node, execute a matrix-vector multiplication to decide which direction to branch.
- **Solution:** March down the tree one level at a time, computing the branches of ALL random walks using batched GEMV / GEMM.



Runtime Benchmarks (LBNL Perlmutter CPU)

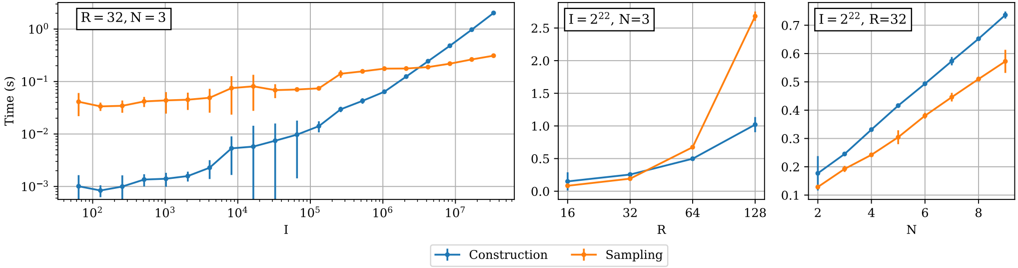


Figure: Time to construct sampler and draw $J = 65,536$ samples. C++ Implementation Linked to OpenBLAS. 1 Node, 128 OpenMP Threads, BLAS3 Construction, BLAS2 Sampling.

Distortion, Ours vs. Approximate Sampling

We define the distortion $D(S, A)$ of sketch S with respect to matrix A by

$$D(S, A) = \kappa(SQ) - 1$$

where Q is any orthonormal basis for the column space of A [Mur+23]. Distortion quantifies the distance preservation property of a sketch.

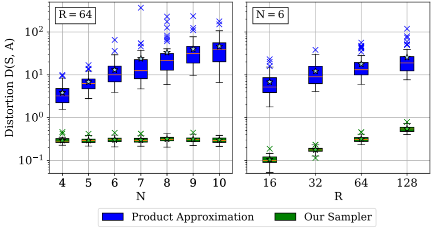


Figure: Sketch distortion as a function of KRP matrix count N and column count R, $J = 65,536$. Green: our sampler. Blue: product approximation by [LK22].

Sparse Tensors from FROSTT

Tensor	Dimensions	NNZ
Uber	$183 \times 24 \times 1.1K \times 1.7K$	$3.3M$
Enron	$6.0K \times 5.6K \times 240K \times 1.2K$	$54M$
NELL-2	$12K \times 9.1K \times 29K$	$77M$
Amazon	$4.8M \times 1.8M \times 1.8M$	$1.7B$
Reddit	$8.2M \times 177K \times 8.1M$	$4.7B$

$$\mathrm{fit}(\tilde{\mathcal{T}}, \mathcal{T}) = 1 - \frac{\left\| \tilde{\mathcal{T}} - \mathcal{T} \right\|_F}{\left\| \mathcal{T} \right\|_F}$$

Accuracy Comparison for Fixed Sample Count

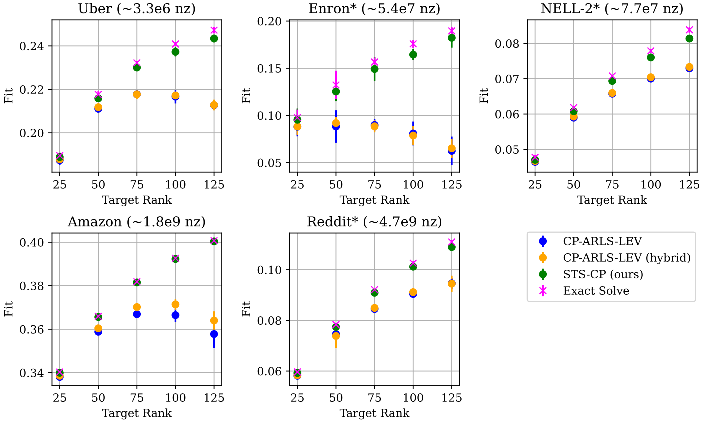


Figure: Sparse tensor ALS accuracy comparison for $J = 2^{16}$ samples, varied target ranks.

STS-CP Makes Faster Progress to Solution

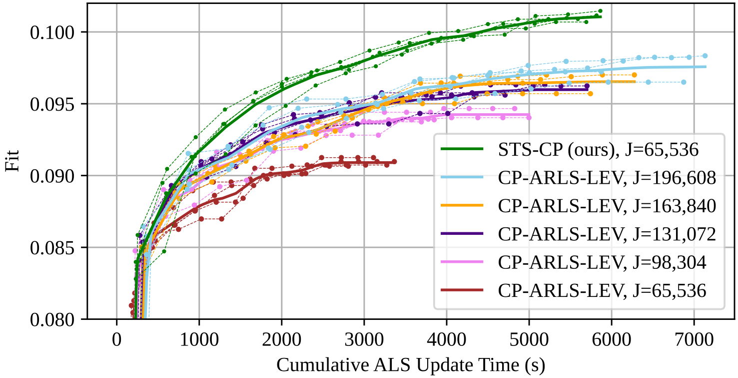
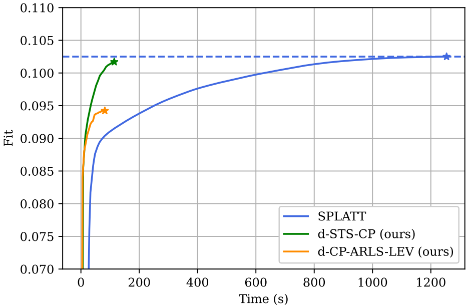


Figure: Fit vs. ALS update time, Reddit tensor, $R = 100$.

Performance at Scale [Bha+24a]



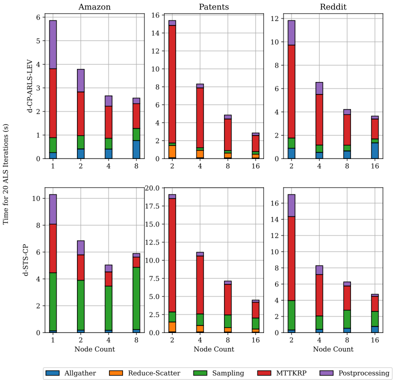


Figure: Fit vs. time, Reddit ($R = 100$) and strong scaling ($R = 25$) for our randomized algorithms.

Conclusions and References

Summary

- We exploited structure in the Khatri-Rao Product to build a leverage score sampler with low polynomial complexity.
- Our implementation relies on well-optimized dense linear algebra primitives, exhibiting strong practical performance in addition to our theoretical guarantees.
- This year, we extended our results to **tensor-train** core chains (find our poster at NeurIPS 2024!) by making key adaptations to our conditional-sampling procedure [Bha+24b].
- Try our code online: `https://github.com/vbharadwaj-bk/fast_tensor_leverage`.

Questions?

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