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Randomized Leverage Score Sampling and CP Decomposition at Scale

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Introduction

The Berkeley BeBOP and PASSION Groups

I am affiliated 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 **randomized algorithms** and **sparse computations** that can be parallelized and deployed at **supercomputer scale**.

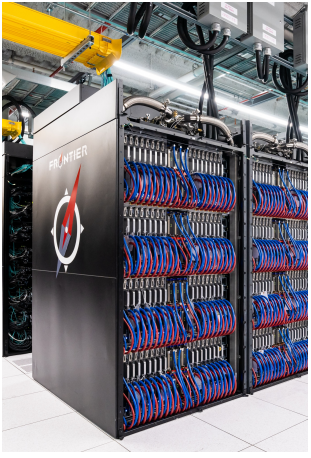


Figure 1: Frontier, the first exascale supercomputer in the United States. Credit: OLCF, Wikimedia Commons CC2.0.

Topics We Will Cover

Today, we will cover two works that use randomization to accelerate sparse tensor CP decomposition. This is a condensed version of my qualifying exam talk, online at:

https://vivek-bharadwaj.com/pdf/2024/qual_slides.pdf.

1. Sketching linear least-squares problems in sparse Candecomp / PARAFAC (Neurips'23; [**Bh**MMGBD23]).

2. Distributed-memory randomized CP methods (Preprint, Arxiv; [**Bh**MMBD23]).

These works are collaborations with Osman Asif Malik, who spoke last week.

Fast Exact Leverage Score Sampling from Khatri-Rao Products

The Khatri-Rao Product

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

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

- 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 $U_j \in \mathbb{R}^{I_j \times R}$.

Motivating Application

This least-squares problem is the computational bottleneck in alternating least-squares Candecomp / PARAFAC (CP) decomposition [KB09].

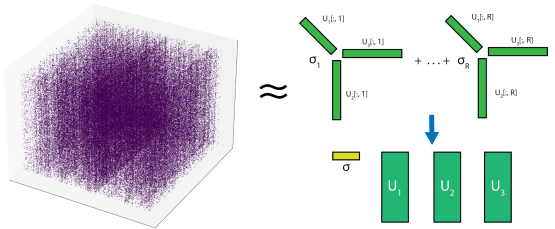


Figure 2: Subregion of Amazon sparse tensor and illustrated CP decomposition.

Focus on large sparse tensors (mode sizes in the millions) and moderate decomposition rank $R \approx 10^2$. Assume $I_j = I$ for all j and $I \geq R$.

Randomized Linear Least-Squares

- **Sketch & Solve**: Apply short-wide sketching matrix S to both A and B, solve reduced problem

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

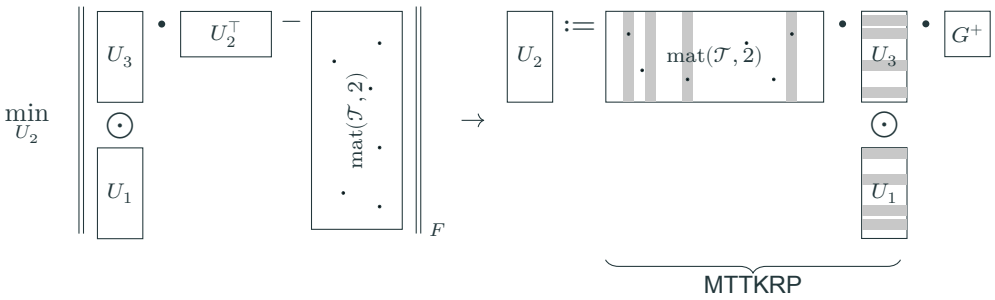
- Want an (ε, δ) guarantee on solution quality: with high probability $(1-\delta)$,

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

- Restrict S to be a *sampling* matrix: selects and reweights rows from A and B. **How do we downsample a Khatri-Rao product accurately AND efficently?**

Effect of Sampling Operator, Sparse Tensor Decomposition

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



Our Contributions [BhMMGBD23]

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 (and even greater advantages for sparse tensors).

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.

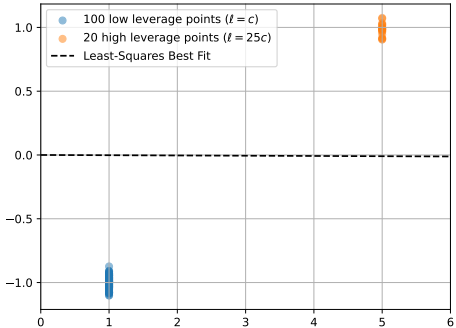
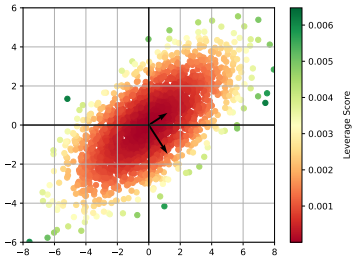


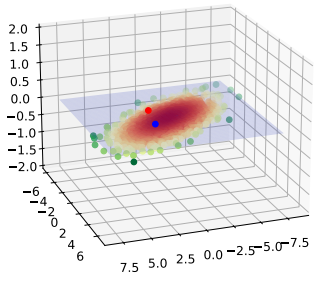
Figure 3: A univariate regression problem with low and high leverage points (intercept constrained to be 0).

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 4: 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 $(0, 0)$).

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. 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.

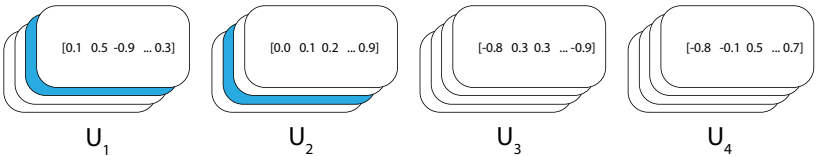
- (CP-ARLS-LEV [LK22]): Similar approximation, hybrid random-deterministic sampling strategy and practical improvements.

- (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.**

Implicit Leverage Score Sampling

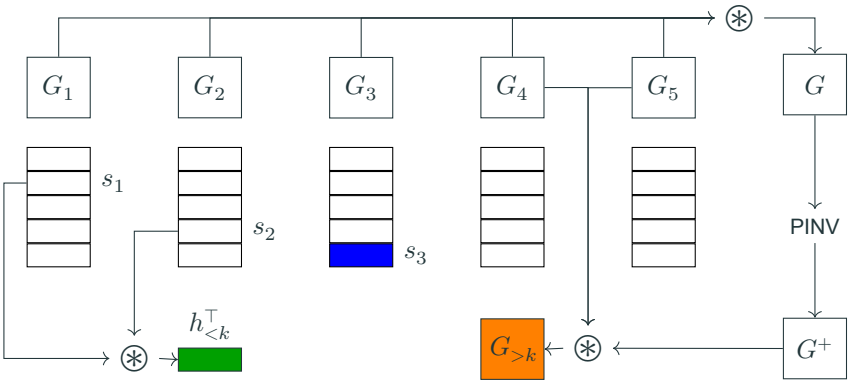
- For $I = 10^7, N = 3$, matrix A has 10^{21} rows. Can't even index rows with 64-bit integers. Instead: use identity $\ell_i = A[i,:](A^\top A)^+ A[i,:]^\top$.

- 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 $\hat{s}_k$



Theorem

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

Key Sampling Primitive

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

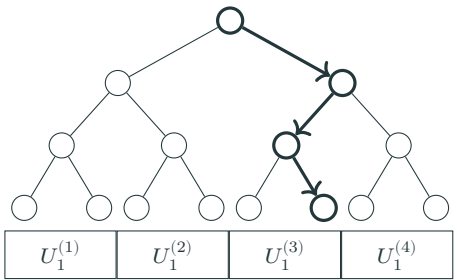
- Can't compute q entirely - would cost $O(IR^2)$ per sample per mode.
- Imagine we magically had all entries of q - how to sample? Initialize I bins, j'th has width $q[j]$.
- Choose random real r in $[0, 1]$, find "containing bin" i such that

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

Binary Tree Inversion Sampling

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

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



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

Caching Partial Gram Matrices

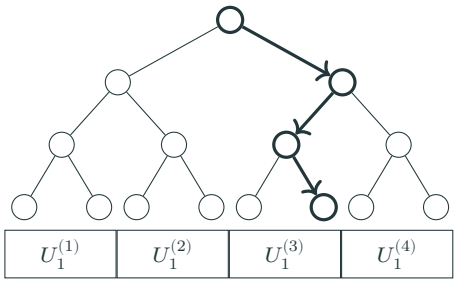
Let an internal node v correspond to an interval of rows $[S(v)...E(v)]$.

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

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

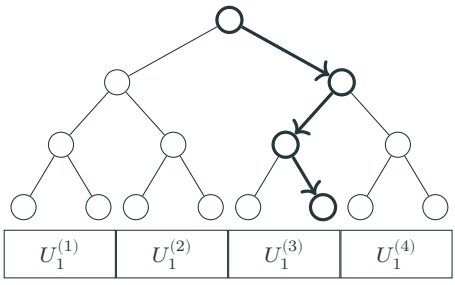
- At internal nodes, compute $C^{-1}\langle h_{<k} h_{<k}^{\top}, G^{v}, G_{>k}\rangle$ in $O(R^2)$ time (read normalization constant from root)
- At leaves, spend $O(R^3)$ time to compute remaining values of q. Can reduce to $O(R^2 \log R)$, see paper.
- Complexity per sample: $O(NR^2 \log I)$ (summed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



High-Performance Parallel Sampling, Approach 1

- 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.

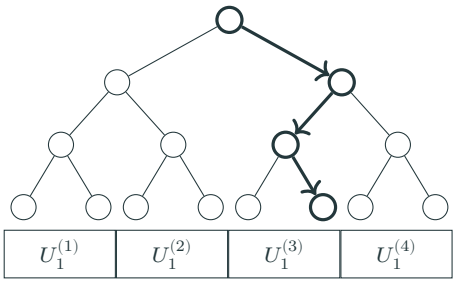
- **Approach 1:** Assign a thread team to execute random walks independently. **Proudly parallel, no data races.**



High-Performance Parallel Sampling, Approach 2

- Issues: irregular memory access pattern on CPU, not optimal for a single GPU thread to execute a BLAS call.

- **Approach 2:** March down the tree one level at a time, computing the branches of ALL random walks with a **batched GEMV / GEMM**.



Runtime Benchmarks (LBNL Perlmutter CPU)

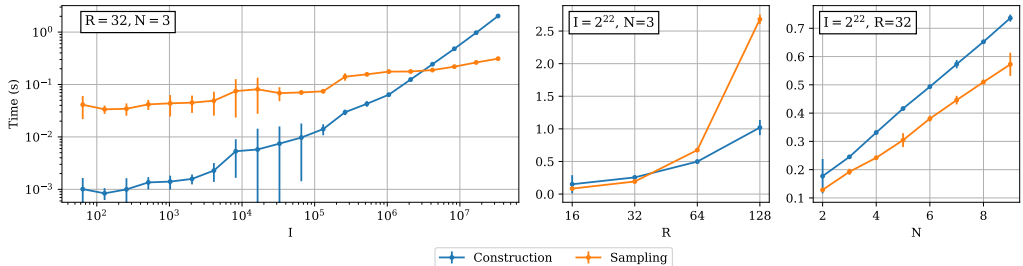


Figure 5: Time to construct sampler and draw $J = 65,536$ samples. C++ Implementation Linked to OpenBLAS. 1 Node, 128 OpenMP Threads, BLAS3 Construction, BLAS2 Sampling.

Distortion, Ours vs. Approximate Leverage Score Sampling

The distortion $D(S, A)$ of sketch S with respect to matrix A is given by

$$D(S, A) = \frac{\kappa(SQ) - 1}{\kappa(SQ) + 1}$$

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

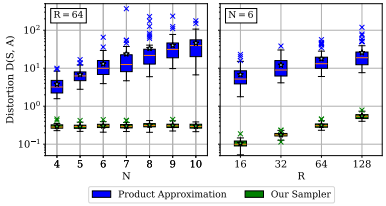


Figure 6: Sketch distortion as a function of KRP matrix count N and column count R, $J = 65,536$. Green: our sampler. Blue: product approximation by [LK22].

Accuracy Comparison for Fixed Sample Count

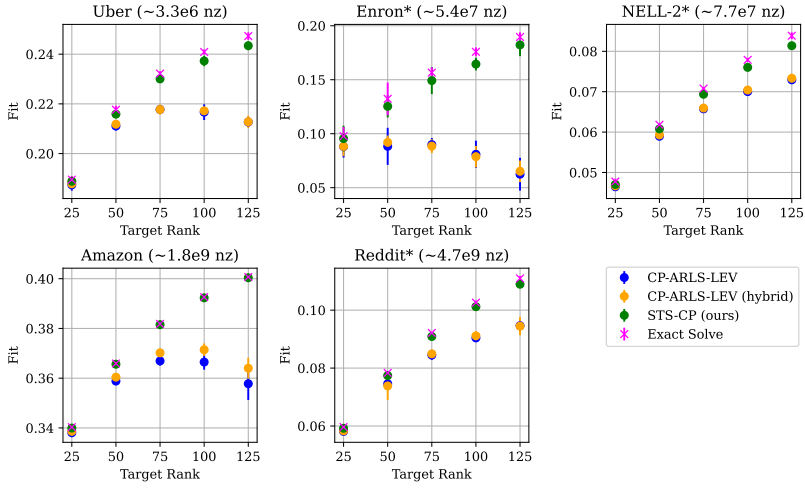


Figure 7: Sparse tensor ALS accuracy comparison for $J = 2^{16}$ samples, varied target ranks.

STS-CP Makes Faster Progress to Solution

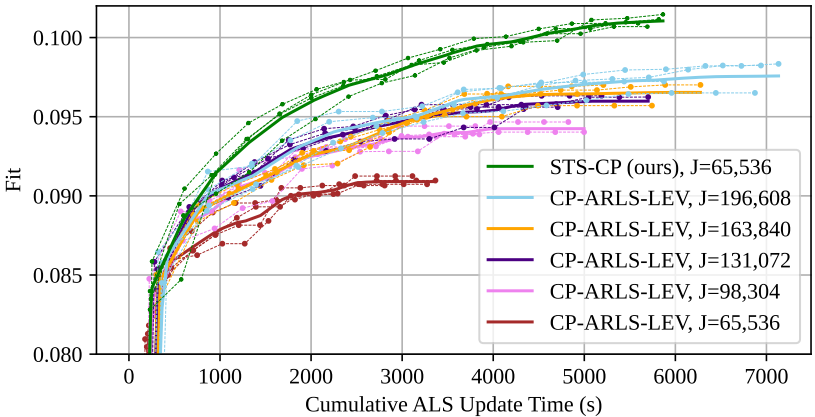


Figure 8: Fit vs. ALS update time, Reddit tensor, $R = 100$.

Takeaways: Faster Leverage Score Sampling from Khatri-Rao Products

- We accelerated sampling from the Khatri-Rao product by devising a novel data structure and a high-performance implementation.
- We demonstrated convincing speedups and accuracy benefits over CP-ARLS-LEV [LK22], an algorithm that approximates the leverage scores.
- **Up next**: distributed-memory formulations of both our algorithm and CP-ARLS-LEV.

High-Performance Randomized CP Decomposition at Scale

Sparse Tensors from FROSTT

Tensor	Dimensions	NNZ
Uber	$183 \times 24 \times 1.1K \times 1.7K$	$3.3M$
Amazon	$4.8M \times 1.8M \times 1.8M$	$1.7B$
Patents	$46 \times 239K \times 239K$	$3.6B$
Reddit	$8.2M \times 177K \times 8.1M$	$4.7B$

- Sparse tensors may have **billions** of nonzero entries, mode sizes in the **tens of millions** [Smi+17].
- Randomized algorithms okay in shared-memory, but **existing codes cannot compete** with classic distributed-memory implementations [Smi+15; Kan+12].

Our Contributions [BhMMBD23]

- We give high-performance implementations of STS-CP and CP-ARLS-LEV scaling to thousands of CPU cores.
- Up to 11x speedup over SPLATT.
- Several communication / computation optimizations unique to randomized CP decomposition.

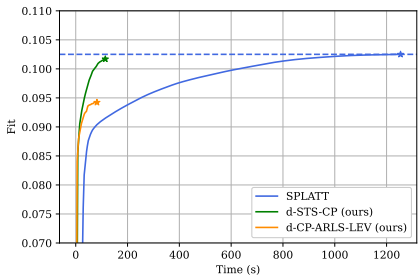


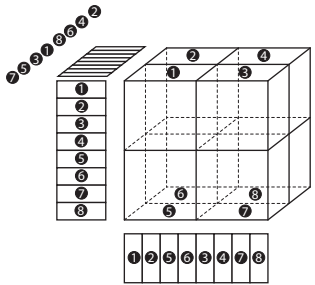
Figure 9: Accuracy vs. time, Reddit tensor, $R = 100$, 512 cores / 4 Perlmutter CPU nodes, 4.7 billion nonzeros.

Methodology

- We distribute STS-CP and CP-ARLS-LEV [LK22] with very distinct communication / computation patterns, each with varying time / accuracy tradeoffs.
- We tailor the communication schedule to randomized CP decomposition to eliminate Reduce-scatter collectives, achieving better load balance in the process.
- We use a hybrid of CSC format for nonzero lookups and CSR format to enable race-free thread parallelism. Key primitive: sparse transpose.

Factor and Sparse Matrix Layout

- Processors arranged in a hypercube.
- Factor matrices $U_1, ..., U_N$ distributed by block rows. Assume that all processors redundantly compute $U_j^\top U_j$ for all j (product is gram matrix G of A).
- Each processor owns a block of the sparse tensor. Randomly permute modes to load-balance.



Bulk-Synchronous Randomized ALS Update

1. **Sampling and All-gather:** Sample rows of $U_{\neq j}$, Allgather the rows to processors who require them.

2. **Local Computation:** Extract the corresponding nonzeros from the local tensor, execute the downsampled MTTKRP.

3. **Reduction and Postprocessing:** Reduce the accumulator of the sparse-dense matrix multiplication across processors, if necessary, and post-process the factor.

Distribution of Distinct Sampling Algorithms

Sampler	Compute	Messages	Words Communicated
d-CP-ARLS-LEV	JN/P	P	P
d-STS-CP	$JR^2 \log I/P$	$P \log P$	$JR \log P/P$

- CP-ARLS-LEV *approximates* the leverage scores with lower computation / communication overhead. Accuracy degrades at high rank.
- STS-CP samples from the *exact* leverage score distribution, requiring higher sampling time.
- **Problem:** How to sample when factors distributed by block rows?

d-CP-ARLS-LEV

- **Key Idea:** Approximate the leverage scores of A by the *product* of leverage scores on each factor matrix U_i.

- Let $U_i^{(p_j)}$ be the block row of U_i owned by processor p_j. Leverages scores of this block given by

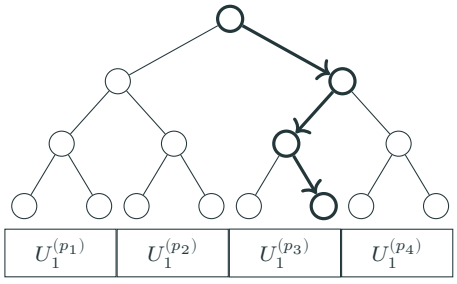
$$\operatorname{diag}\left(U_i^{(p_j)} G^{+} U_i^{(p_j)\top}\right)$$

- Computed locally on each processor without communication. Sampling requires (in expectation) only a small constant number of words communicated.

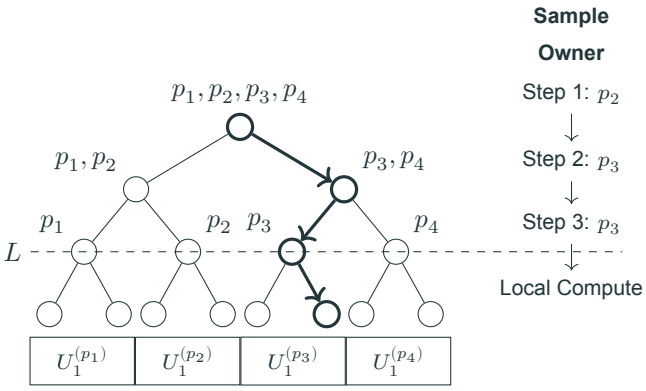
- **Drawback:** Accuracy degrades for high N or R.

d-STS-CP

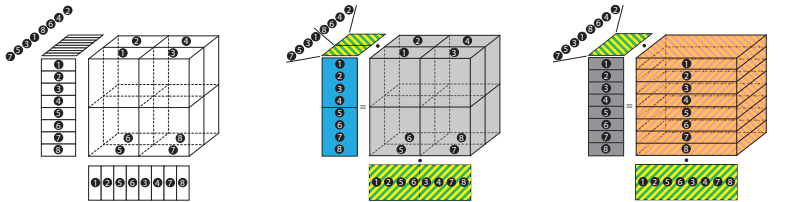
- Samples from **exact** leverage score distribution by sampling from each of $U_1, ..., U_N$ in sequence (excluding U_j).
- Execute random walk on binary tree to find the row index for each U_j. Node v caches "partial Gram matrix " G^v.
- At each node, compute $h^\top G^v h$ (where h is unique to each sample) to decide whether to branch left / right.



d-STS-CP Parallelization Scheme

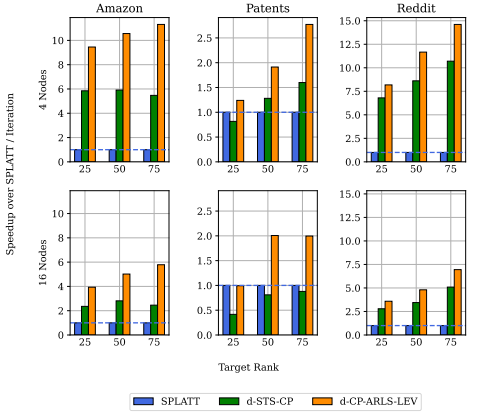


Randomization-Tailored Communication Schedule

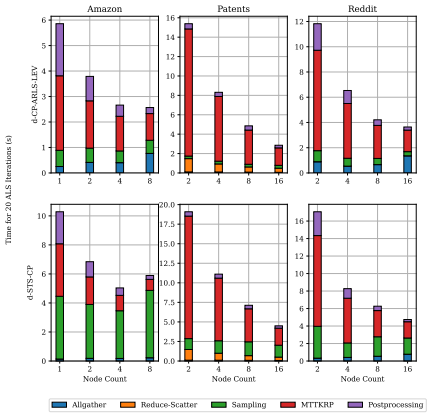


Schedule	Words Communicated / Round
Non-Randomized TS	$2NR\left(\prod_{k=1}^{N} I_k/P\right)^{1/N}$
Sampled TS	$NR\left(\prod_{k=1}^{N} I_k/P\right)^{1/N}$
Sampled AS	$JRN(N-1)$

Speedup and Scaling on Large Sparse Tensors



(a) Speedup



(b) Strong Scaling, $R = 25$

Figure 10: Speedup over SPLATT and strong scaling for our randomized algorithms.

Comparison of Communication Schedules

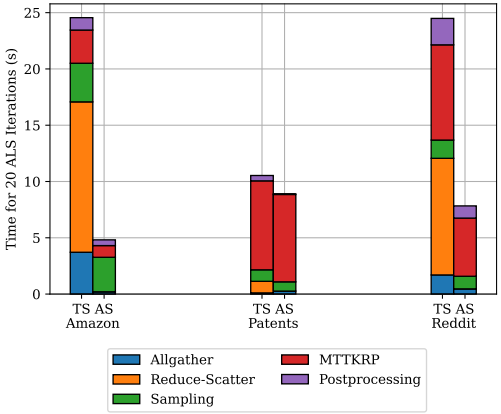


Figure 11: Runtime breakdown for tensor-stationary vs. accumulator-stationary communication schedules.

Takeaways: Distributed-Memory Randomized CP Algorithms

- We proposed the first distributed-memory implementation of two sampling-based, sparse CP algorithms.
- We optimized our algorithms to avoid communication in both the sampling and MTTKRP phases.
- Our method scales to thousands of CPU cores with significant speedups over existing SOTA sparse tensor decomposition software.

Questions? View slides, other material on my website:

`https://vivek-bharadwaj.com`

References i

[**Bh**MMBD23] Vivek Bharadwaj, Osman Asif Malik, Riley Murray, Aydin Buluç, and James Demmel. ***Distributed-Memory Randomized Algorithms for Sparse Tensor CP Decomposition.*** 2023. arXiv: *2210.05105 [math.NA]*.

[**Bh**MMGBD23] Vivek Bharadwaj, Osman Asif Malik, Riley Murray, Laura Grigori, Aydın Buluç, and James Demmel. **"Fast Exact Leverage Score Sampling from Khatri-Rao Products with Applications to Tensor Decomposition".** In: *Thirty-seventh Conference on Neural Information Processing Systems*. Dec. 2023.

[Che+16] Dehua Cheng, Richard Peng, Yan Liu, and Ioakeim Perros. **"SPALS: Fast Alternating Least Squares via Implicit Leverage Scores Sampling".** In: *Advances in Neural Information Processing Systems*. Vol. 29. Curran Associates, Inc., 2016.

[DKM06] Petros Drineas, Ravi Kannan, and Michael W. Mahoney. **"Fast Monte Carlo Algorithms for Matrices I: Approximating Matrix Multiplication".** In: *SIAM Journal on Computing* 36.1 (2006), pp. 132–157. doi: *10.1137/S0097539704442684*.

References ii

[DM20] Michal Derezinski and Michael W. Mahoney. **“Determinantal Point Processes in Randomized Numerical Linear Algebra”.** In: *CoRR* abs/2005.03185 (2020). arXiv: *2005.03185*.

[Kan+12] U. Kang, Evangelos Papalexakis, Abhay Harpale, and Christos Faloutsos. **“GigaTensor: scaling tensor analysis up by 100 times - algorithms and discoveries”.** In: *Proceedings of the 18th ACM SIGKDD international conference on Knowledge discovery and data mining*. KDD ’12. New York, NY, USA: Association for Computing Machinery, Aug. 2012, pp. 316–324. isbn: 978-1-4503-1462-6.

[KB09] Tamara G. Kolda and Brett W. Bader. **“Tensor Decompositions and Applications”.** In: *SIAM Review* 51.3 (Aug. 2009). Publisher: Society for Industrial and Applied Mathematics, pp. 455–500. issn: 0036-1445. doi: *10.1137/07070111X*.

[LK22] Brett W. Larsen and Tamara G. Kolda. **“Practical Leverage-Based Sampling for Low-Rank Tensor Decomposition”.** In: *SIAM Journal on Matrix Analysis and Applications* 43.3 (2022), pp. 1488–1517.

References iii

[Mal22] Osman Asif Malik. **"More Efficient Sampling for Tensor Decomposition With Worst-Case Guarantees".** In: *Proceedings of the 39th International Conference on Machine Learning*. Vol. 162. Proceedings of Machine Learning Research. PMLR, July 2022, pp. 14887–14917.

[Min+23] Rachel Minster, Irina Viviano, Xiaotian Liu, and Grey Ballard. **"CP decomposition for tensors via alternating least squares with QR decomposition".** In: *Numerical Linear Algebra with Applications* 30.6 (2023), e2511. doi: *https://doi.org/10.1002/nla.2511*.

[MS22] Linjian Ma and Edgar Solomonik. **"Cost-efficient Gaussian tensor network embeddings for tensor-structured inputs".** In: *Advances in Neural Information Processing Systems*. Vol. 35. Curran Associates, Inc., 2022, pp. 38980–38993.

[Mur+23] Riley Murray, James Demmel, Michael W. Mahoney, N. Benjamin Erichson, Maksim Melnichenko, Osman Asif Malik, Laura Grigori, Piotr Luszczek, Michal Derezinski, Miles E. Lopes, Tianyu Liang, Hengrui Luo, and Jack Dongarra. ***Randomized Numerical Linear Algebra: A Perspective on the Field With an Eye to Software*.** Tech. rep. UCB/EECS-2023-19. EECS Department, University of California, Berkeley, Feb. 2023.

References iv

[Smi+15] Shaden Smith, Niranjay Ravindran, Nicholas D. Sidiropoulos, and George Karypis. **"SPLATT: Efficient and Parallel Sparse Tensor-Matrix Multiplication".** In: *2015 IEEE International Parallel and Distributed Processing Symposium*. ISSN: 1530-2075. May 2015, pp. 61–70.

[Smi+17] Shaden Smith, Jee W. Choi, Jiajia Li, Richard Vuduc, Jongsoo Park, Xing Liu, and George Karypis. ***FROSTT: The Formidable Repository of Open Sparse Tensors and Tools*.** 2017. url: `http://frostt.io/`.

[Woo14] David P. Woodruff. **"Sketching as a Tool for Numerical Linear Algebra".** In: *Found. Trends Theor. Comput. Sci.* 10.1–2 (Oct. 2014), pp. 1–157. issn: 1551-305X.

Backup Slides, Deck 1: Fast Khatri-Rao Product Leverage Score Sampling

Leverage Score Sampling Proof Sketch

Theorem (Structural Conditions for LSTSQ, [DKM06])

*Let Q be a basis for the column-space of A. Suppose that a sketching matrix S satisfies the following two **deterministic** structural conditions:*

- ***(S1) Approximate Isometry**: $\sigma_{min}(SQ) \geq 1/\sqrt{2}$*
- ***(S2) Minimal Junk**: $\left\|Q^\top S^\top S B^\perp\right\|_F^2 \leq \varepsilon \left\|B^\perp\right\|_F^2 / 2$*

Then the sketched solution $\tilde{X}$ satisfies

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

Main Proof Idea: Show, with probability $\geq (1-\delta)$, that a leverage score sketch satisfies these two conditions.

Leverage Score Sampling Proof Sketch

- (S1) holds by the well-known ℓ_2-subspace embedding property of leverage score sketches [Woo14], with probability $\geq 1 - \delta/2$ for high enough sample count.

- (S2) holds by an approximate matrix-multiplication argument [DKM06] (with one-sided information) with probability $\geq 1 - \delta/2$.

$$\begin{aligned} \left\|Q^\top S^\top S B^\perp\right\|_F^2 &= \left\|\mathbf{0} - Q^\top S^\top S B^\perp\right\|_F^2 \\ &= \left\|Q^\top B^\perp - Q^\top S^\top S B^\perp\right\|_F^2 \end{aligned}$$

- Use a union bound to guarantee that both hold with probability $\geq 1 - \delta$. Will sketch the proof of (S1).

Leverage Score Sampling Gives an ℓ_2-SE Proof Sketch

Proof follows a version by David Woodruff (we adapt it to our notation and drop the β parameter). Let $A = Q\Sigma V^\top$; we need a matrix Chernoff result.

Theorem (Matrix Chernoff, [Woo14])

Let $X_1, ..., X_J$ be independent copies of a symmetric random matrix $X \in \mathbb{R}^{R\times R}$ satisfying

1. $E[X] = 0$,
2. $\|X\|_2 \leq \gamma$,
3. $\left\|E\left[X^\top X\right]\right\|_2 \leq T \leq J^2$.

Let $W = \frac{1}{J}\sum_{i=1}^{J} X_i$. Then for any $\tilde{\varepsilon} > 0$,

$$Pr\left[\|W\|_2 > \tilde{\varepsilon}\right] \leq 2R\exp\left(-J\tilde{\varepsilon}^2/(2T + 2\gamma\tilde{\varepsilon}/3)\right)$$

Leverage Score Sampling Gives an ℓ_2-SE Proof Sketch

Want to show, for appropriate parameters J, γ, ε, that $\frac{1}{\sqrt{2}} \leq \sigma_i^2(SU)$ w.h.p. $(1-\delta)$. Let $z_i = (SU)_{i:}^\top$, $q_j = Q_{j:}^\top$ and choose

$$p_j := \ell_j / R \quad \forall j$$

$$X_i := I - z_i z_i^\top / p_i$$

$$\gamma := 1 + R$$

$$\tilde{\epsilon} := 1 - 1/\sqrt{2}$$

$$T := R - 1$$

Easy to verify that $\mathrm{E}[X] = 0$, need to check conditions (2) and (3) of the Chernoff bound.

Leverage Score Sampling Gives an ℓ_2-SE

Condition 2: $\|X\|_2 \leq \gamma$ implies $\max_{j\in[I]} \left\|I - \frac{q_j q_j^\top}{p_j}\right\| \leq \gamma$. For any j, we have

$$\begin{aligned}
\left\|I - \frac{q_j q_j^\top}{p_j}\right\|_2 &\leq \|I\|_2 + \left\|\frac{q_j q_j^\top}{p_j}\right\|_2 \\
&= 1 + \frac{R\|q_j q_j^\top\|_2}{\|q_j\|_2^2} \\
&= 1 + R \\
&= \gamma
\end{aligned}$$

Crucially, this choice for p_j allows the **minimal** choice $1 + R$ for γ.

Leverage Score Sampling Gives an ℓ_2-SE

Condition 3: We derive

$$\begin{aligned}
\mathrm{E}\left[X^\top X\right] &= \sum_{j=1}^{I} p_j (I - q_j q_j^\top / p_j)(I - q_j q_j^\top / p_j) \\
&= \sum_{j=1}^{I} p_j I - 2 \sum_{j=1}^{I} p_j q_j q_j^\top / p_j + \sum_{j=1}^{I} \frac{p_j q_j q_j^\top q_j q_j^\top}{p_j^2} \\
&= I - 2I + \sum_{j=1}^{I} \frac{q_j q_j^\top q_j q_j^\top}{p_j} \\
&= I - 2I + \sum_{j=1}^{I} R q_j q_j^\top \\
&= (R-1)I
\end{aligned}$$

So $\left\|\mathrm{E}\left[X^\top X\right]\right\|_2 = R - 1 \leq J^2$.

Leverage Score Sampling Gives an ℓ_2-SE

Evaluating the Chernoff guarnatee, we ignore $\tilde{\epsilon}$ since it is a constant. We **want**

$$\exp\left(-J\tilde{\varepsilon}^2/(2T + 2\gamma\tilde{\varepsilon}/3)\right) \leq \delta$$
$$J/(2R + 2R/3)) \geq \Omega\left(\log\frac{R}{\delta}\right)$$

Setting $J = \Omega\left(R \log \frac{R}{\delta}\right)$ causes the failure probability to fall below the threshold.

The Normal Equations in Tensor Decomposition

- The normal equations are widely used for ALS CP decomposition [KB09] despite squaring the condition number.

- QR decomposition of a KRP is more difficult to compute (but only slightly) [Min+23]:

$$\begin{aligned} A &:= U_1 \odot ... \odot U_N \\ &= (Q_1 R_1) \odot ... \odot (Q_N R_N) \\ &= (Q_1 \otimes ... \otimes Q_N) \cdot (R_1 \odot ... \odot R_N) \\ &= (Q_1 \otimes ... \otimes Q_N) \cdot Q_{\text{tail}} \cdot R_{\text{tail}} \end{aligned} \tag{2}$$

- QR formulation useful for lower-precision decomposition, adversarial tensors [Min+23], e.g. $\sin(x_1 + ... + x_N)$.

Why Don’t We Use the QR Formulation?

- QR Decomposition not useful for leverage score sampling. R^N samples required to sketch $Q_1 \otimes ... \otimes Q_N$, computation of Q_{tail} introduces exponential cost in N.
- Leverage score computation robust to numerical error (just take slightly more samples).
- For our applications, we can sacrifice some accuracy.

Backup Slides, Deck 2: Randomized Distributed CP Decomposition

d-STS-CP Parallelization Scheme

- Matrices G^v replicated $\log P$ times. Each processor stores data on path from leaf to root.
- **Initialization:** Each sample assigned arbitrarily to a processor (along with corresponding sample vectors h).
- **At Each Node:** Branching decision made for each sample, Alltoallv computed to reorganize sample vectors.
- **Drawback:** Repeated Alltoallv calls are expensive!

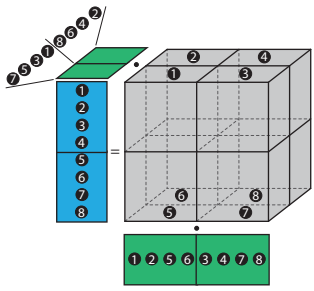
Non-Randomized Communication Analysis

- Let processor grid dimensions be $P_1 \times ... \times P_N$.
- All-gather + Reduce-Scatter Costs:

$$2\sum_{k=1}^{N} IR/P_k$$

- Cost Under Optimal Grid:

$$\frac{2NRI}{P^{1/N}}$$

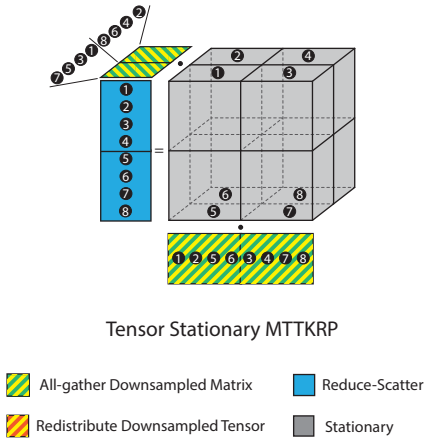


Downsampled Tensor-Stationary MTTKRP

- Reduce-scatter cost is unchanged by sampling.
- Minimum communication:

$$\frac{NRI}{P^{1/N}}$$

- Drops at most a constant factor compared to non-randomized ALS

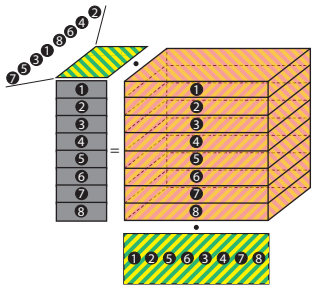


Downsampled Accumulator-Stationary MTTKRP

- Eliminate reduce-scatter by gathering sampled rows to all processors, redistributing sampled nonzeros.
- Communication Cost:

$$JRN(N-1) + \frac{3}{P}\sum_{j=1}^{N} \text{nnz}(\text{mat}(\mathcal{T}, j)S_j^\top).$$

- Avoid retransmitting nonzeros by storing N different matricizations of the tensor.

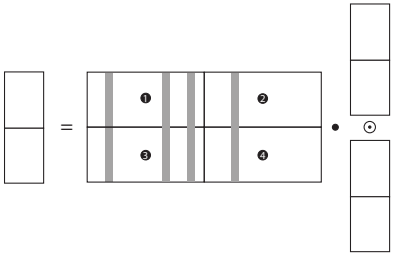


Accumulator Stationary MTTKRP

All-gather Downsampled Matrix
Reduce-Scatter
Redistribute Downsampled Tensor
Stationary

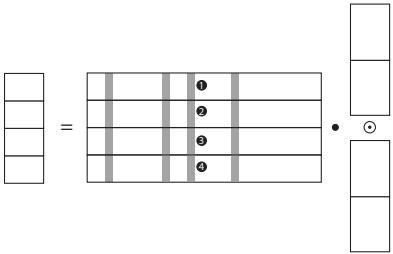
Tensor-Stationary MTTKRP Load Balance

- We use random permutations of each tensor mode to evenly distribute nonzeros & samples to processors.
- Theoretical model: each sampled column has q nonzeros with row i.i.d. uniform.
- TS Load Balance: J balls into $P^{1-1/N}$ bins (each ball here is a column).



Accumulator-Stationary MTTKRP Load Balance

- AS Load Balance: Jq balls into P bins.
- Here, each ball is a nonzero entry. This distibution has better load balance when q is high.



Load Balance

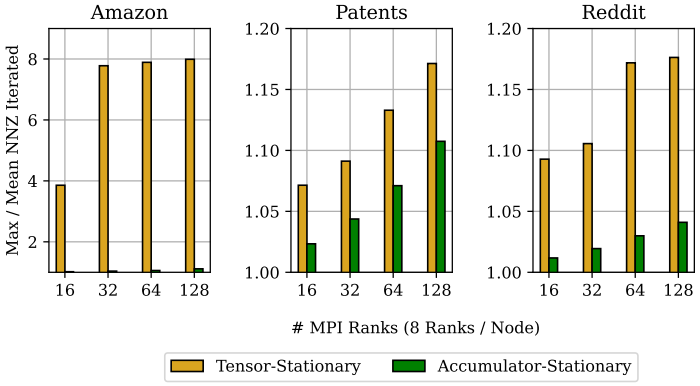
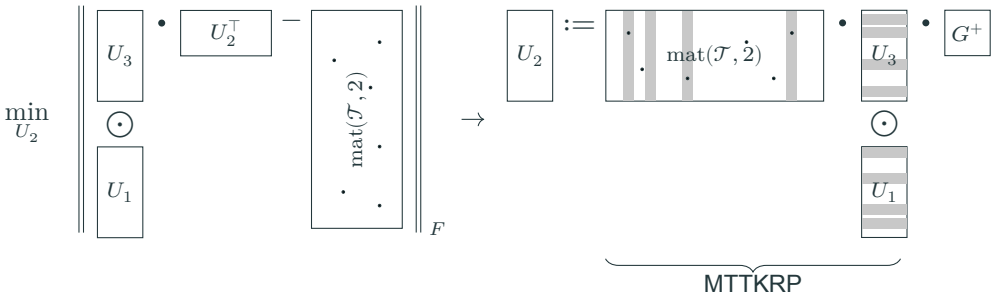


Figure 12: Load imbalance for tensor-stationary vs. accumulator stationary schedules as a function of MPI rank count.

Local Computation: SpMTTKRP is SpMM

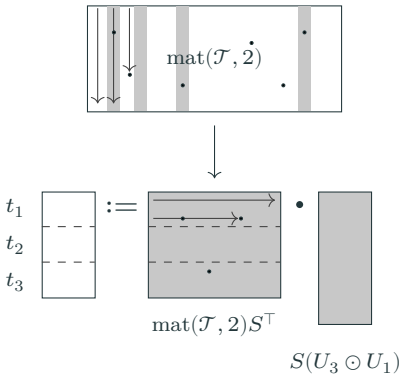
$$\min_{U_j} \left\| \left[\bigodot_{k \neq j} U_k \right] \cdot U_j^\top - \text{mat}(\mathcal{T}, j)^\top \right\|_F$$



Matricized Tensor Storage Format

- **CSC**: Easy to look up nonzeros, but need atomics when accumulating to output buffer (with multiple threads)
- **CSR:** No data races, but difficult to select nonzeros.
- **Solution:** Use CSC for lookup, sparse transpose into CSR.

Sampling and Sparse Transpose Operation



Drawback: Need to store N copies of the sparse tensor, but we do this anyway to avoid communication.

Weak Scaling

- **Weak scaling for non-randomized CP**: increase target rank R and processor count proportionally, measure runtime.

- **Problems for Randomized CP:**
  - Nonzero count selected from sparse tensor varies.
  - Need higher sample counts at higher ranks to maintain accuracy.

- **Solution:** Benchmark STS-CP with fixed sample count to maintain accuracy (as much as possible) for a fixed sample count, measure throughput instead:

$$\text{Throughput} = \frac{\text{nnz selected in MTTKRP}}{\text{Runtime}}$$

Experimental Platform

- Experiments conducted on up to 16 nodes / 2048 CPU cores on NERSC Perlmutter at LBNL.
- Hybrid OpenMP / MPI implementation in C++, Python wrappers using Pybind11.
- Baseline : SPLATT, a highly-optimized CP decomposition library.

Figure 13: LBNL Perlmutter, an HPE Cray Supercomputer (#12 on the Nov'23 Top500).

Weak Scaling

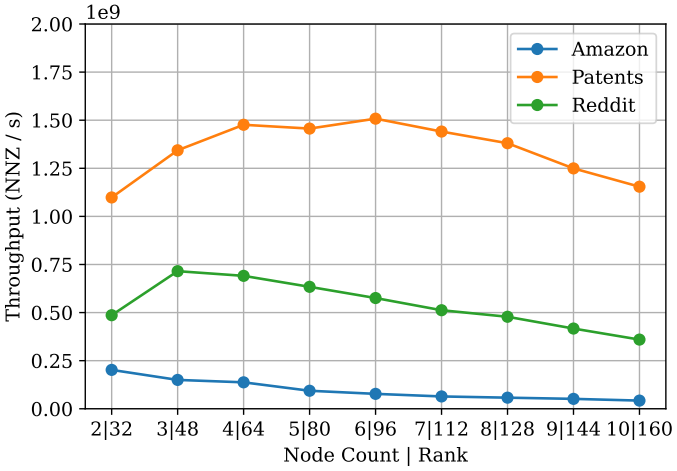


Figure 14: Throughput as a function of increasing target rank and node count.