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Exploiting Sparsity and Randomness to Accelerate Linear Least-Squares at Scale

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Date & Time: January 17, 2024, 12pm PST

Location: Room 510, Soda Hall

Introduction

Bedrock: Dense Linear Algebra

- Many algorithms in machine learning and scientific computing rely on linear algebraic (LA) primitives.
- BLAS [Law+79] & LAPACK [And+92]: Enabled non-specialists to use optimized dense LA kernels.
- SCALAPACK [Bla+97], MAGMA [TDB10], SLATE [Gat+20] & many others: Extended capabilities to massively parallel architectures and accelerators.

Figure 1: Frontier, the first US exascale machine. Credit: OLCF at ORNL, Wikimedia Commons CC2.0.

Sparsity Introduces New Challenges

Consider a linear least-squares problem of the form $\min_X \|AX - B\|_F$. What happens if:

- A or B has **structural sparsity** (most entries are zero)?
- A is **data-sparse** (written as a Kronecker product, or related structure)?
- B is only available *on-demand*, and we must **induce sparsity** to reduce the sampling complexity?

Dense LA methods are often intractable! Need tailored algorithms and custom computational kernels to achieve high performance.

Randomization in Numerical Linear Algebra

- Randomized computing has a long history. Randomized linear algebra has seen significant progress since 2008 (e.g. [RT08], Blendenpik [AMT10]) [Woo14].

- Key ingredient: **sketching**. Example for overdetermined LSTSQ: apply random matrix S with far fewer rows than columns, solve cheaper problem

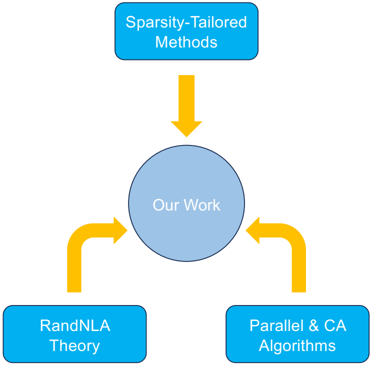
$$\min_X \|SAX - SB\|_F$$

- Efforts are underway to standardize randomized linear algebra primitives [Mur+23]. Intersection of sparsity and RandNLA: open frontier.

High-Level Contributions of this Work

Our goal: accelerate sparse LSTSQ problems using randomization and communication avoiding (CA) parallel algorithms. We will:

- **Identify** applications involving sparse linear least-squares problems.
- **Design** novel randomized techniques and parallelization strategies tailored to that sparsity.
- **Deploy** our methods on parallel architectures at scale.



Topics We Will Cover

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

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

3. CA-algorithms for sparse matrix *completion* (IPDPS'22; [**Bh**BuDe22]).

4. Future work: sketching to accelerate the marginalized graph kernel, emerging extensions of sketching for tensor trains.

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 $A = U_1 \odot ... \odot U_N$ 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].

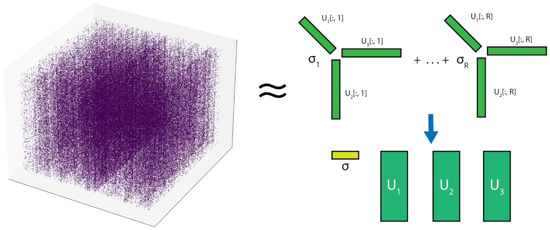


Figure 2: Subregion of Amazon sparse tensor and illustrated CP decomposition.

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

$$\min_{\tilde{X}} \left\| S A \tilde{X} - S B \right\|_F$$

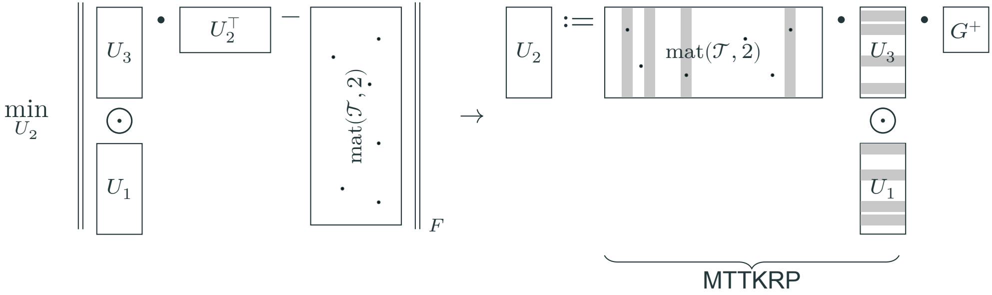
- Want an (ε, δ) guarantee on solution quality: with high probability $(1 - \delta)$,

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

- 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.

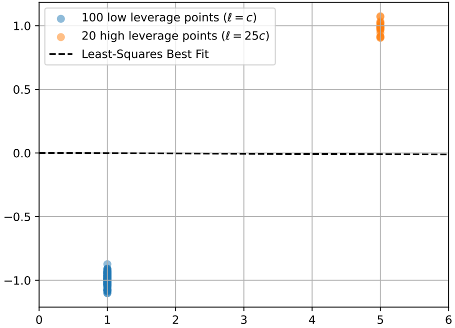
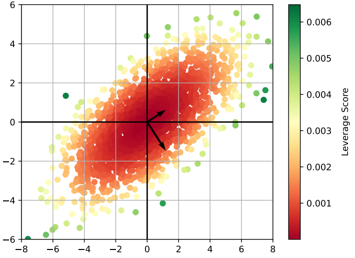


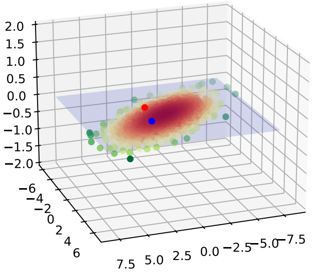
Figure 3: A univariate regression problem with low and high leverage points (intercept constrained to be 0).

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 $x \in \mathbb{R}^R$,

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

- 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

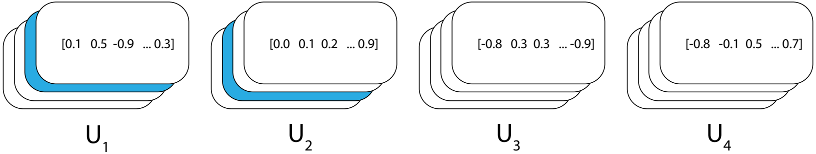
Problem: Cost to compute all leverage scores exactly is identical to runtime of QR decomposition. Defeats the purpose of sampling!

- (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

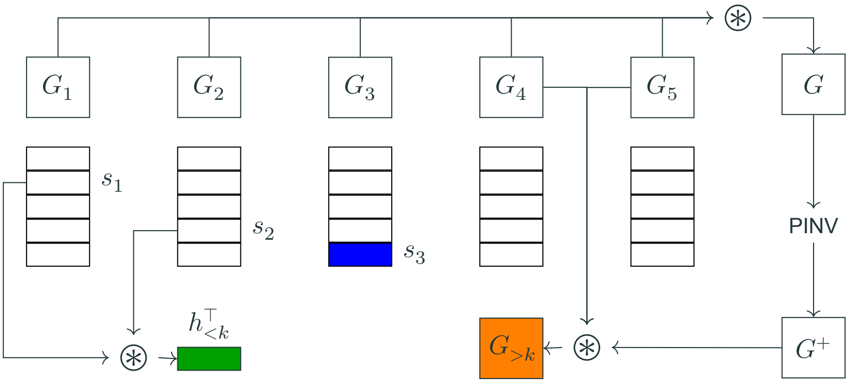
- For $I = 10^7, N = 3$, matrix A has 10^{21} rows. Can't even index rows with 64-bit integers. Instead: use identity $\ell_i = A[i,:] \, (A^\top A)^+ A[i,:]^\top$.

- 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

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

Key Sampling Primitive

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

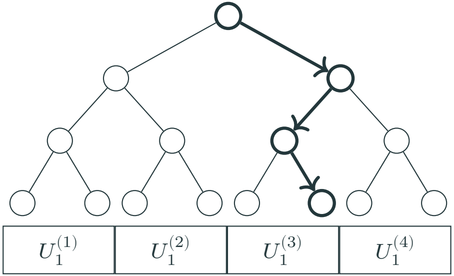
- Can't compute q entirely - would cost $O(IR^2)$ per sample per mode.
- Imagine we magically had all entries of q - how to sample? Initialize I bins, j'th has width $q[j]$.
- Choose random real r in $[0,1]$, find "containing bin" i such that

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

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 $[S(v)...E(v)]$.

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

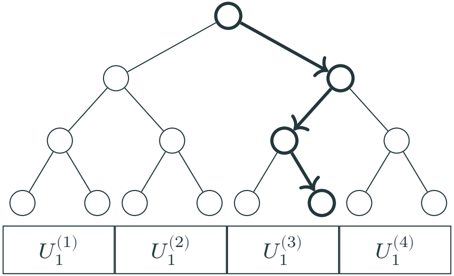
Can compute and store G^v for ALL nodes v in time $O(IR^2)$, storage space $O(IR)$. Use BLAS-3 **syrk** calls in parallel to efficiently construct the tree.

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.

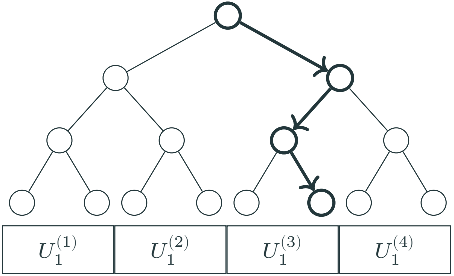
- Complexity per sample: $O(NR^2 \log I)$ (summed over all tensor modes).



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.

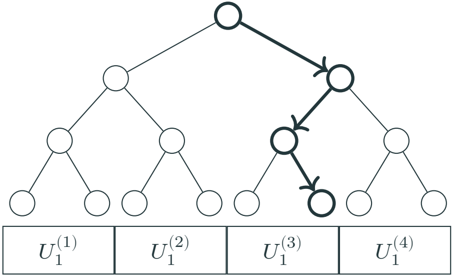
- **Approach 1:** Assign a thread team to execute random walks independently. **Proudly parallel, no data races.**



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)

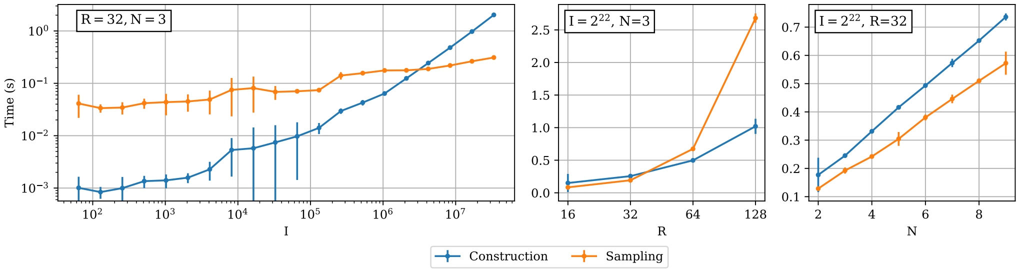


Figure 5: Time to construct sampler and draw $J = 65,536$ samples. C++ Implementation Linked to OpenBLAS. 1 Node, 128 OpenMP Threads, BLAS3 Construction, BLAS2 Sampling.

Distortion, Ours vs. Approximate Leverage Score Sampling

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.

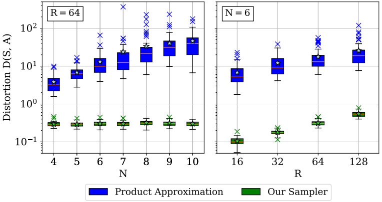


Figure 6: Sketch distortion as a function of KRP matrix count N and column count R, $J = 65,536$. Green: our sampler. Blue: product approximation by [LK22].

Accuracy Comparison for Fixed Sample Count

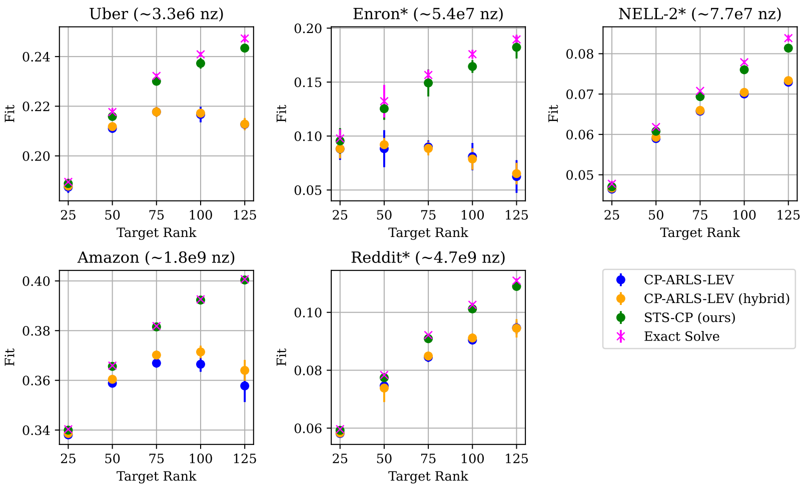


Figure 7: Sparse tensor ALS accuracy comparison for $J = 2^{16}$ samples, varied target ranks.

STS-CP Makes Faster Progress to Solution

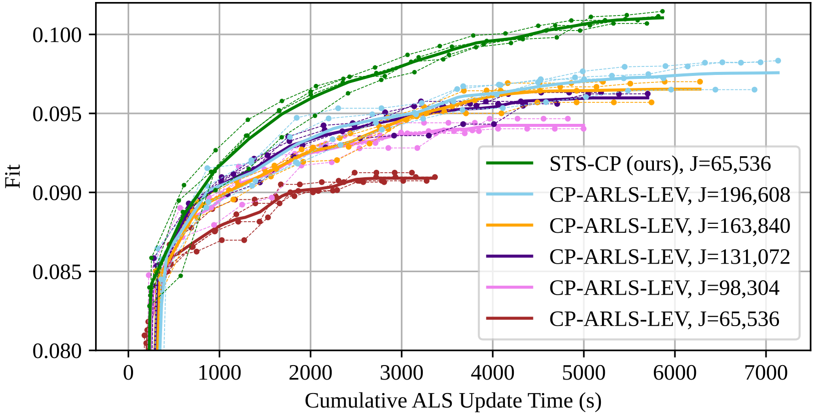


Figure 8: Fit vs. ALS update time, Reddit tensor, $R = 100$.

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.

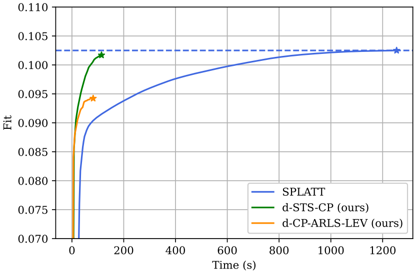


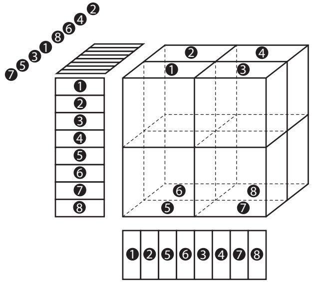
Figure 9: Accuracy vs. time, Reddit tensor, $R = 100$, 512 cores / 4 Perlmutter CPU nodes, 4.7 billion nonzeros.

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	$JR^2 \log I/P$	$P \log P$	$JR \log P/P$

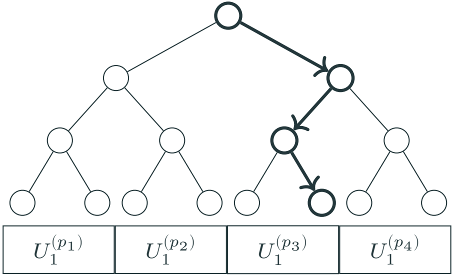
- CP-ARLS-LEV *approximates* the leverage scores with lower computation / communication overhead. Accuracy degrades at high rank.
- STS-CP samples from the *exact* leverage score distribution, requiring higher sampling time.
- **Problem:** How to sample when factors distributed by block rows?

d-CP-ARLS-LEV

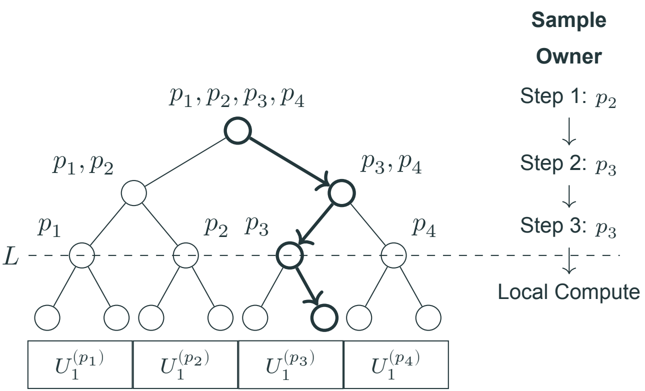
- **Key Idea:** Approximate the leverage scores of A by the *product* of leverage scores on each factor matrix U_i.
- Let $U_i^{(p_j)}$ be the block row of U_i owned by processor p_j. Leverages scores of this block given by
$$\mathrm{diag}\left(U_i^{(p_j)} G^{+} U_i^{(p_j)\top}\right)$$
- Computed locally 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

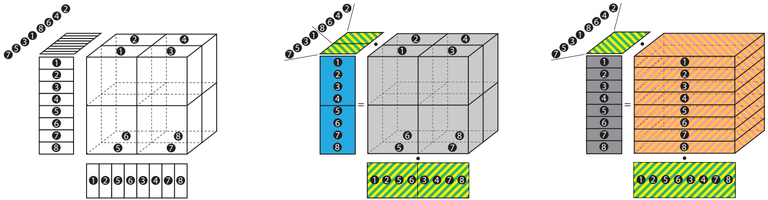
- Samples from **exact** leverage score distribution by sampling from each of $U_1, ..., U_N$ in sequence (excluding U_j).
- Execute random walk on binary tree to find the row index for each U_j. Node v caches "partial Gram matrix" G^v.
- At each node, compute $h^\top G^v h$ (where h is unique to each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



d-STS-CP Parallelization Scheme



Randomization-Tailored Communication Schedule

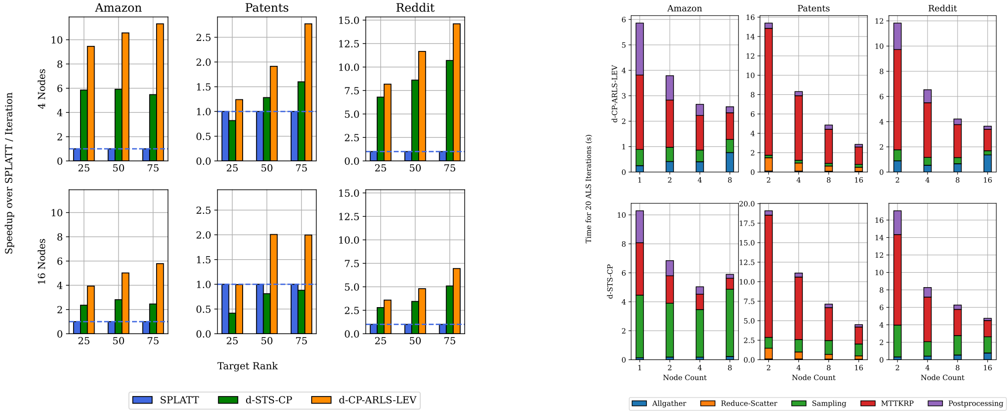


Initial Data Distribution | Tensor Stationary MTTKRP | Accumulator Stationary MTTKRP

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

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

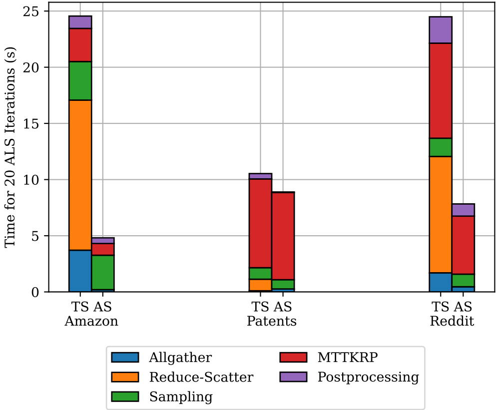


Figure 11: Runtime breakdown for tensor-stationary vs. accumulator-stationary communication schedules.

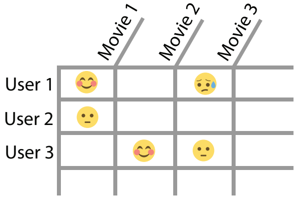
Takeaways: Distributed-Memory Randomized CP Algorithms

- 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.

Communication-Avoiding Algorithms for Matrix Completion

Matrix / Tensor Completion vs. Factorization

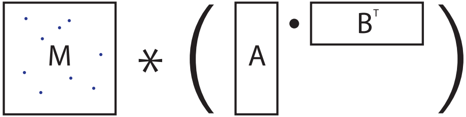
- **Sparse Tensor Completion:** Zero indicates *unobserved data*. Want to fit model only to observed entries, expect it to generalize. Distinct from factorization, where zeros are "true zeros".



- For simplicity, we will focus on the matrix case. Let $S \in \mathbb{R}^{m \times n}$ be the matrix we want to factor and $A \in \mathbb{R}^{m \times r}, B \in \mathbb{R}^{n \times r}$ be embedding matrices.

Collaborative Filtering

- **Factorization:** Solve $\min_{A,B} \left\| S - AB^\top \right\|_F$.
- **Completion:** Solve $\min_{A,B} \left\| S - M \circledast (AB^\top) \right\|_F$, where M is a binary mask with the same sparsity pattern as S.
- $M \circledast (AB^\top)$ is called **sampled dense-dense matrix multiplication**.



ALS Formulation

Cheap, first-pass algorithm (can be modified to impose nonnegativity): alternating least-squares.

- Keep B fixed, solve for A:

$$A := \min_X \left\| M \circledast (XB^\top) - S \right\|_F$$

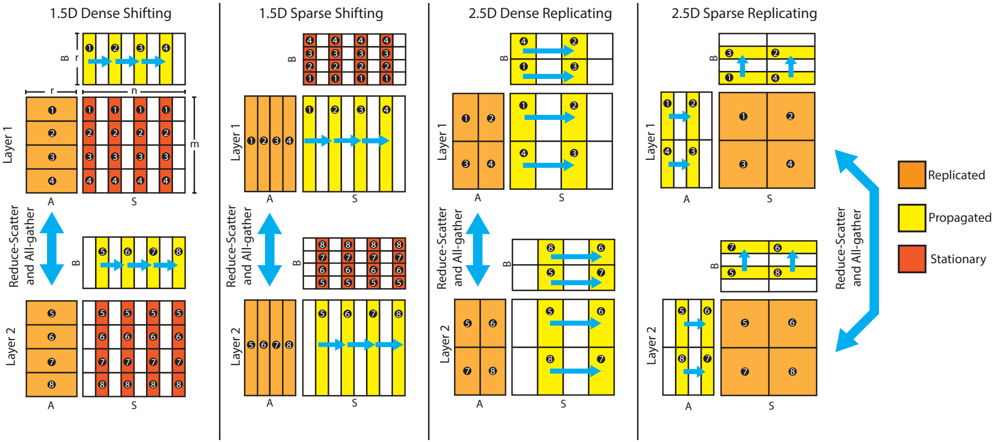
- In standard form, we get an independent LSTSQ problem for each output row of A (each E_j selects nonzero indices of $M[j,:]$):

$$\mathrm{vec}(A) := \mathrm{argmin}_x \left\| \begin{bmatrix} E_1 B & & & \\ & E_2 B & & \\ & & \ddots & \\ & & & E_m B \end{bmatrix} x - \mathrm{vec}_{nz}(S) \right\|_2$$

Our Contributions [BhBuDe22]

- **Prior work:** The ALS algorithm for matrix completion can be reformulated to depend entirely on the SDDMM and SpMM kernels (running in a conjugate-gradient loop) [CZ13; Nis+18].
- We build communication-avoiding, distributed-memory implementations of the SDDMM and SpMM kernels. We use them in sparse matrix factorization on **hundreds** of Cori CPU nodes.
- These can also be used for specific graph neural network architectures with self-attention (similar to CAGNET [TYB20]).

Existing Algorithms for SpMM



SpMM / SDDMM Duality

SDDMM and SpMM have **identical** data access patterns: every nonzero $(i, j) \in \mathrm{nz}(S)$ requires an interaction between row i of A and row j of B.

procedure SpMM(S, B)
  Initialize $A := 0$;
  for $(i, j) \in \mathrm{nz}(S)$ **do**
    $A[i, :] \mathrel{+}= S[i, j]\, B[j, :]$
  return A

procedure SDDMM(S, A, B)
  Initialize $R := 0$;
  for $(i, j) \in \mathrm{nz}(S)$ **do**
    $R[i, j] = S[i, j]\, (A[i, :] \cdot B[j, :])$
  return R

Observation: Every distributed algorithm for SpMM can be converted into an algorithm for SDDMM, and vice-versa.

Converting SpMM Algorithms to SDDMM Algorithms

Consider any distributed algorithm for SpMM that performs no replication. For all $k \in [1, r]$, the algorithm must (at some point)

- Co-locate $S[i,j]$, $A[i,k]$, $B[j,k]$ on a single processor
- Perform the update $A[i,k] \mathrel{+}= S[i,j]\, B[j,k]$

Transform the algorithm as follows:

1. Change the input sparse matrix S to an output initialized to 0.
2. Change A from an output to an input.
3. Have each processor execute the local update $S[i,j] \mathrel{+}= A[i,k]\, B[j,k]$

Dealing with Replication

Inputs are typically replicated via broadcasts, outputs via reduction. To handle this:

- Replace initial braodacasts of inputs with terminal reductions.
- Replace terminal reductions of outputs with initial broadcasts.

The resulting algorithm performs SDDMM up to multiplication with the original values in S.

We performed a communication analysis for several variants of SpMM / SDDMM, as well as optimizations that fuse the two kernels back-to-back.

Strong Scaling on LBNL Cori

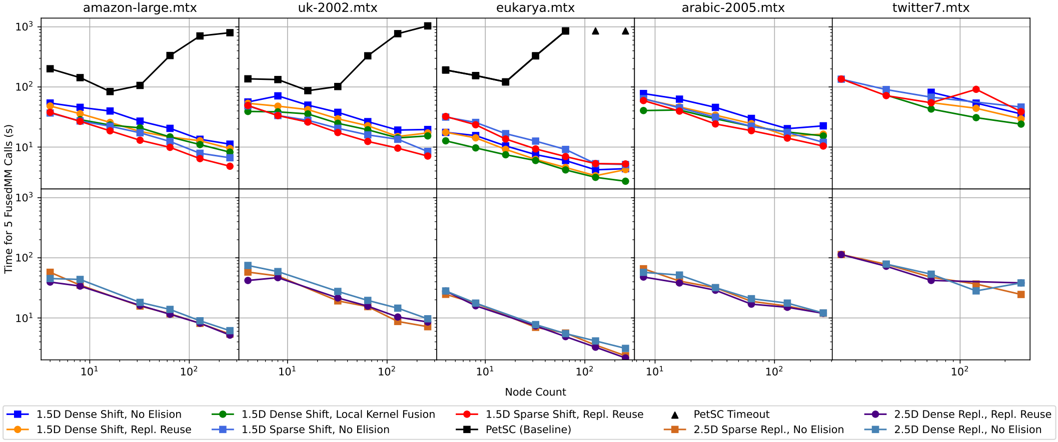


Figure 12: Strong scaling Experiments for 5 back-to-back SDDMM and SpMM calls on Cori CPU nodes.

Applications: Collaborative Filtering and GATs

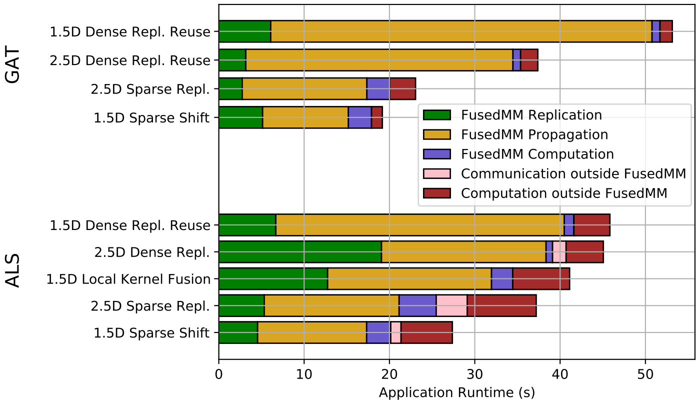


Figure 13: Application benchmarks for our distributed SDDMM / SpMM implementations

Takeaways: Communication Avoiding SDDMM / FusedMM Kernels

- We devised a procedure to convert well-analyzed SpMM algorithms into SDDMM algorithms.
- We analyzed the communication costs of a pair of back-to-back SpMM / SDDMM calls and demonstrated significant speedups at scale over the implementation in PETSc.
- We used our methods to accelerate ALS matrix completion on some of the largest matrices in the Suitesparse collection.

Future Work

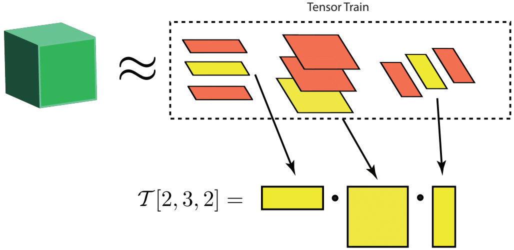
Work in Progress

Currently exploring three thrusts:

- Extensions of our CP sampling strategy to other tensor formats (mainly tensor trains).
- Application of sketching to domain science problems, such as Electrical Impedence Tomography (EIT).
- Accelerating other problems that involve tensor product structure, such as the marginalized graph kernel.

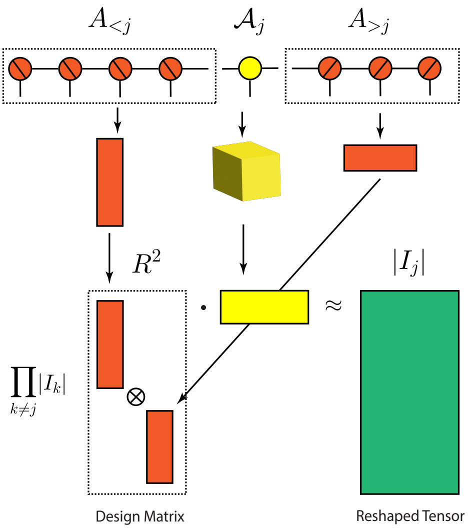
Extension of Implicit Sampling to Tensor Train Decomposition

The tensor-train decomposition represents a tensor $\mathcal{T}$ as a contraction between order-3 "tensor-cores".



j'th core has dimensions $R_j \times I_j \times R_{j+1}$. Represents a tensor with I^N elements using $O(NIR^2)$ space when all rank are equal.

Iterative TT Optimization Problems



Sampling from $A_{<j}$

Theorem (Orthonormal Subchain Leverage Sampling)

There exists a data structure that costs $O(IR^3)$ per tensor train core to build / update. For any $1 < j \leq N$, the structure can sample a row from $A_{<j}$ proportional to its squared row norm in time

$$O((j-1)R^2 \log I)$$

Apply same binary tree trick to the left matricizations of each core $\mathcal{A}_j$, exploit orthonormality to reduce complexity. Accelerates TT-ALS, potentially useful in other contexts.

Tensor Structure in PDE-Inverse Problems

Consider a 2D slice of conducting tissue. A source voltage is applied and the potential is measured at several pairs of boundary points.

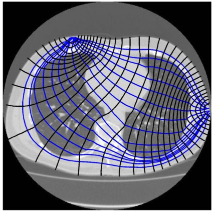
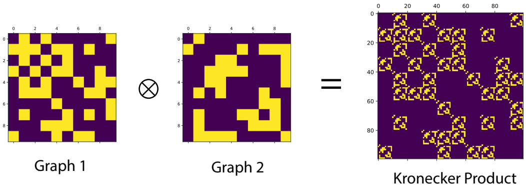


Figure 14: CT Image of thorax with EIT equipotential lines. Image credit Andy Adler, CC3.0 unported, Wikimedia Commons.

Goal: determine conductivity in **interior** of tissue. Solve $(U_{11} \odot U_{12} + U_{21} \odot U_{22})x = b$ where $U_{11}, U_{12}, U_{21}, U_{22}$ depend on the geometry of the tissue / boundary, b is a measurement taken for every source / sink pair [Che+20].

Sketching for the Marginalized Graph Kernel

The marginalized graph kernel computes a similarity measure between two (labeled, weighted) graphs G_1, G_2 by finding the stationary distribution of a random walk on their **Kronecker Product Graph** [Vis+10].



For the **inner product edge kernel**: solve $\left(\sum_{i=1}^{N} A_i \otimes B_i\right) x = p$ where A_i, B_i have the sparsity structures of adjacency matrices of A_1, A_2. Potentially a ripe application for Tensorsketch, low-rank approximation.

Conclusions and Acknowledgements

Summary

- We exhibited algorithms for ALS CP decomposition that have **lower asymptotic complexity and faster time-to-solution** compared to SOTA competitors.
- We showed that randomized methods are practical on **thousands of CPU cores** and **billion-scale sparse tensors**, offering up to 11x speedup over carefully-engineered deterministic algorithms
- We optimized the SDDMM kernel involved in sparse matrix factorization based on proven algorithms for SpMM, exploiting **algorithmic duality** between the two kernels.
- Planned work this year: investigate other regression problems that involve tensor structure, particularly scientific applications.

Acknowledgements

This slide will expand to a whole section in my dissertation talk! For now, my appreciation goes to:

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- Collaborators Laura Grigori, Osman Asif Malik, Riley Murray.
- Committee members Katherine Yelick and Michael Lindsey.
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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 $X_1, \ldots, X_J$ 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

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

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

$$\gamma := 1 + R$$

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

$$T := R - 1$$

Easy to verify that $\mathrm{E}\left[X\right] = 0$, 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

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

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

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]:

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

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

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!

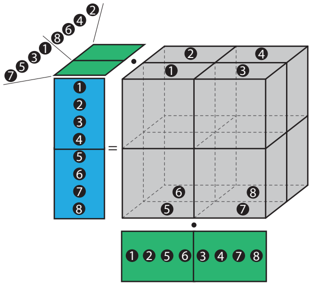
Non-Randomized Communication Analysis

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

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

- Cost Under Optimal Grid:

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



Tensor Stationary MTTKRP

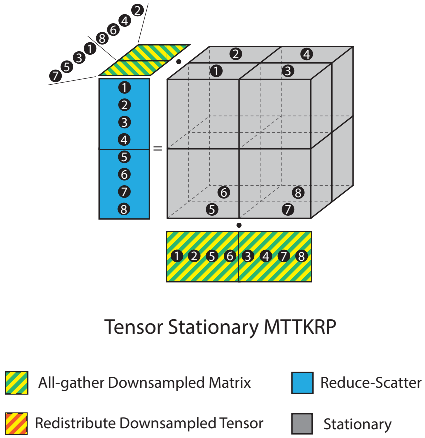
All-gather Matrix
Reduce-Scatter
Redistribute Downsampled Tensor
Stationary

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



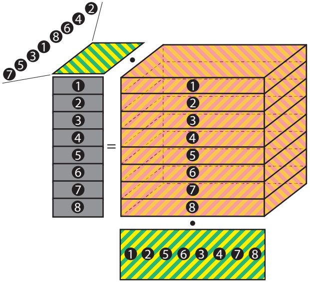
Downsampled Accumulator-Stationary MTTKRP

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

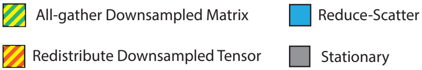
- Communication Cost:

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

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

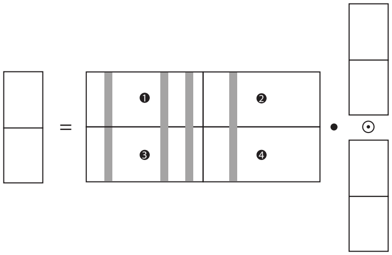


Accumulator Stationary MTTKRP



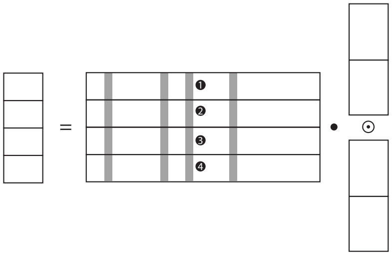
Tensor-Stationary MTTKRP Load Balance

- 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

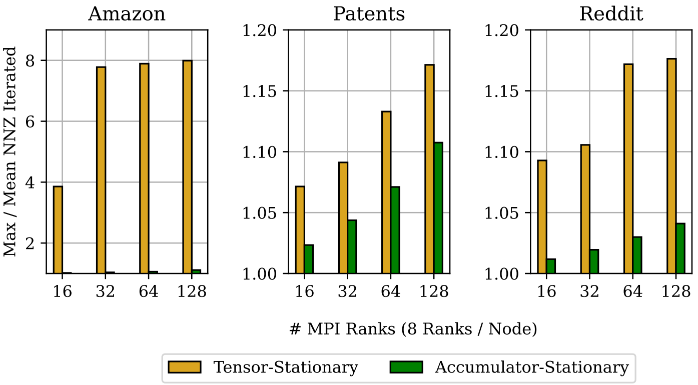
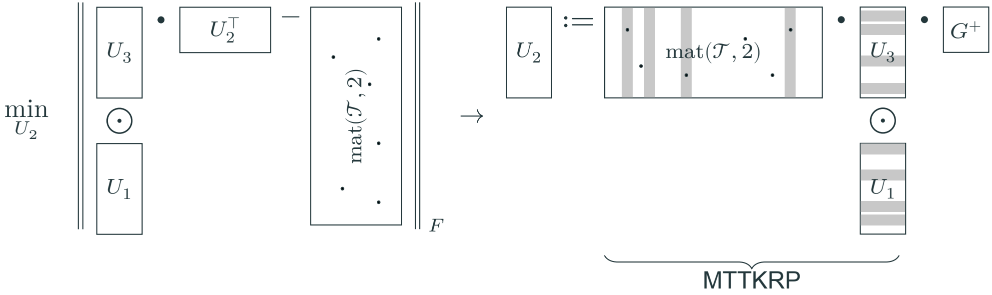


Figure 15: Load imbalance for tensor-stationary vs. accumulator stationary schedules as a function of MPI rank count.

Local Computation: SpMTTKRP is SpMM

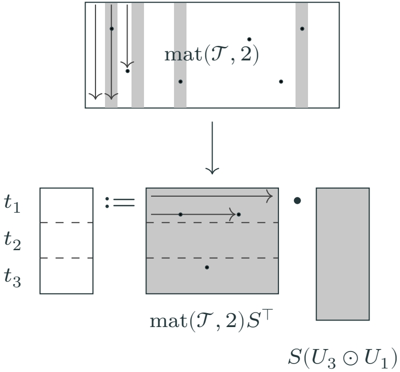
$$\min_{U_j} \left\| \left[\bigodot_{k\neq j} U_k \right] \cdot U_j^\top - \mathrm{mat}(\mathcal{T}, j)^\top \right\|_F$$



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 16: LBNL Perlmutter, an HPE Cray Supercomputer (#12 on the Nov’23 Top500).

Weak Scaling

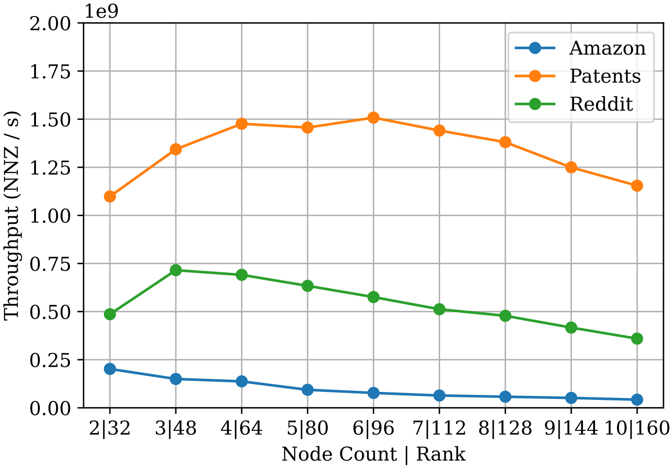


Figure 17: Throughput as a function of increasing target rank and node count.