Randomized Algorithms for Tensor Decompositions in the Tucker Format

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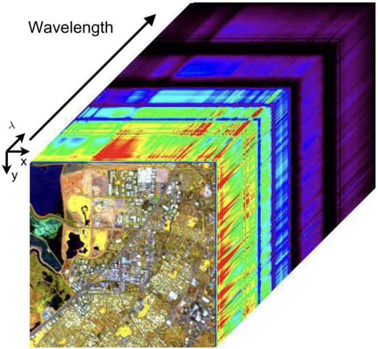
Acknowledgements to NSF CCF 1942892 for funding

Motivation: Multidimensional data

Multidimensional data appears in many applications:

- Numerical simulations for PDE's
- Facial recognition
- Hyperspectral imaging



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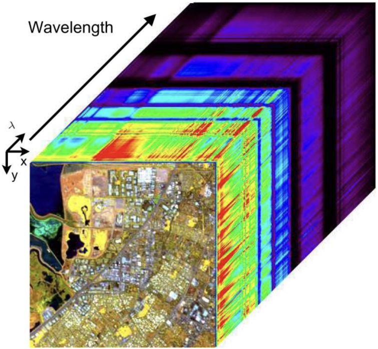

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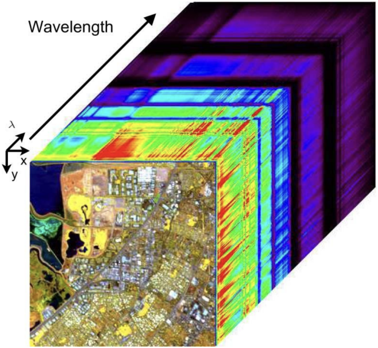

Goal: efficiently obtain compressed representation of data

Method: use parallel, randomized algorithms for Tucker decompositions

- can obtain large compression ratios with high accuracy

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Contributions

- New parallel, randomized algorithms for computing the Tucker decomposition
  - Uses a Kronecker product of random matrices to exploit structure
  - Significantly reduces computational cost compared to deterministic and randomized counterparts

Minster, Li, Ballard, *Parallel Randomized Tucker Decomposition Algorithms*, arXiv:2211.13028

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- New parallel method of computing a multi tensor-times-matrix (multi-TTM) product, an "all-at-once" approach
  - Reduces communication compared to previous approaches

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- New parallel method of computing a multi tensor-times-matrix (multi-TTM) product, an "all-at-once" approach
  - Reduces communication compared to previous approaches
- Theoretical error bound for the algorithms

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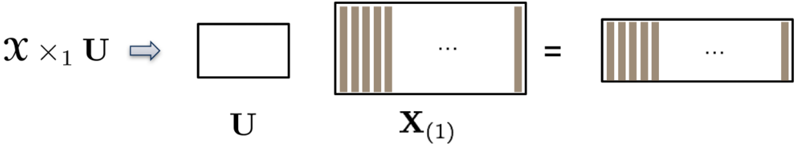
Outline

1. Background
   1. Key tensor operations
   2. Tucker format
   3. Randomized range finder
2. Randomized Tucker algorithms
   1. Sequential algorithms
   2. Error Analysis
   3. Accuracy experiments
3. Parallel approach
4. Numerical results

Key tensor operations:

- Tensor-times-matrix (TTM): $\mathcal{X} \times_j U$
  - Tensor multiplied by a matrix in a single mode j
  - Computed as matrix multiplication: matrix times unfolded tensor



Tensor-times-matrix (TTM) and Multi-TTM

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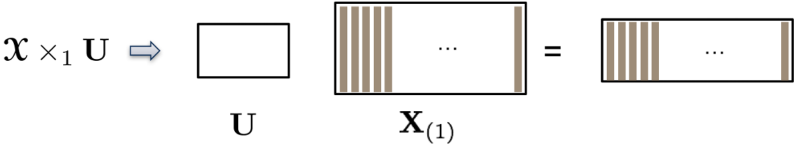


- Multi-TTM: $\mathcal{X} \times_1 U_1 \times_2 U_2 \cdots \times_d U_d$ for d-mode tensor
  - Can be unfolded in j-th mode as

$$U_j X_{(j)} (U_d \otimes U_{d-1} \otimes \cdots \otimes U_{j+1} \otimes U_{j-1} \otimes \cdots \otimes U_1)^\top$$

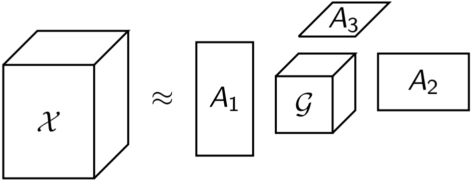
with $\otimes$ the Kronecker product

Tucker Format

Approximates tensor $\mathcal{X}$ as

$$\mathcal{X} \approx \mathcal{G} \times_1 A_1 \times \cdots \times_d A_d$$

with $\mathcal{G} \in \mathbb{R}^{r_1 \times \cdots \times r_d}$, $A_j \in \mathbb{R}^{n_j \times r_j}$



Popular algorithms: Higher Order SVD (HOSVD)[1] and Sequentially Truncated Higher Order SVD (STHOSVD)[2]

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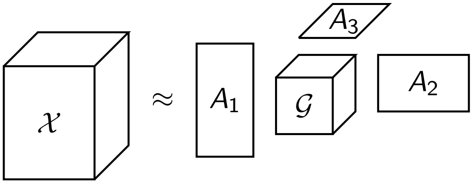

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General approach:

1. Unfold tensor along mode j
2. Compute rank-r_j SVD of mode unfolding
3. Factor matrix A_j formed from left singular vectors
4. Core (or partial core) formed via TTM's

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Our approach:

- Use a randomized algorithm[3] to speed up SVD step
  - Use a Kronecker product of random matrices instead of single random matrix to exploit structure
- Implement in parallel
  - Use a new, faster parallel version of a key operation (multi-TTM) to significantly lower runtime

[3] Ahmadi-Asl, Abukhovich, Asante-Menash, Chichocki, Phan, Tanaka, Oseledets, IEEE Access, 2021

Randomized Range Finder

For a matrix X, finds a matrix Q that estimates the range of X, or $X \approx QQ^\top X$

Inputs: matrix $X \in \mathbb{R}^{m \times n}$
target rank $r \leq \operatorname{rank} X$
oversampling parameter p

Main Steps:

1. Draw $\Omega \in \mathbb{R}^{n \times (r+p)}$, a random matrix
2. Form product $Y = X\Omega$
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Idea: Use Kronecker product of k random matrices Φ_j as $\Omega = \Phi_1 \otimes \Phi_2 \otimes \cdots \otimes \Phi_k$ so that

$$Y = X\Omega = X(\Phi_1 \otimes \Phi_2 \otimes \cdots \otimes \Phi_k)$$

takes the form of an unfolded multi-TTM

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Randomized HOSVD with Kronecker Product

Inputs: $\mathcal{X} \in \mathbb{R}^{n\times\cdots\times n}$, target rank $(r, \ldots, r)$, oversampling parameter p

Main steps:

For modes $j = 1 : d$,

1. **Randomized range finder of unfolding $X_{(j)}$**
   a. Compute $Y_{(j)} = X_{(j)}\Omega$ via Multi-TTM in all modes but j:

   $$\mathcal{Y} = \mathcal{X} \times_1 \Phi_1^{(j)} \times \cdots \times_{j-1} \Phi_{j-1}^{(j)} \times_{j+1} \Phi_{j+1}^{(j)} \times \cdots \times_d \Phi_d^{(j)}$$

   b. Thin QR of $Y_{(j)} = A_j R$ with $A_j \in \mathbb{R}^{n\times(r+p)}$

End for

3. Form core via multi-TTM: $\mathcal{G} = \mathcal{X} \times_1 A_1^\top \times \cdots \times_d A_d^\top$
4. Truncate down to target rank
   a. Deterministic HOSVD on $\mathcal{G}$, combine factor matrices with A_j's

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Comparison: algorithm types

Standard approach: one random matrix $\Omega \in \mathbb{R}^{n^{d-1}\times(r+p)}$

- Computing $Y = X_{(1)}\Omega \quad \rightarrow \quad$ one large matrix multiply

Our approach: Kronecker product of random matrices $\Omega = \Phi_2 \otimes \cdots \otimes \Phi_d$ with $\Phi_j \in \mathbb{R}^{n\times s}$, $s^{d-1} = r + p$

- Computing $Y = X_{(1)}\Omega \quad \rightarrow \quad$ one multi-TTM with skinny matrices

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Two options for our approach:

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1. Use an independent product of Φ_j's per mode
2. Reuse same Kronecker factors Φ_j in Ω_j for each mode
   - Allows for reuse of computations
   - Makes analysis more complicated

Error Analysis for R-Kron, RST-Kron, R-Kron-reuse

Parameters:

- d-way tensor $\mathcal{X} \in \mathbb{R}^{n \times n \times \cdots \times n}$
- target rank $(r, r, \ldots, r)$, oversampling parameter p
- $\alpha, \beta > 1$ satisfying $n > r + p \geq \frac{\alpha^2 \beta}{(\alpha-1)^2}(r^2 + r)$
- SRHT random matrices: $\Phi = DH$
  - D diagonal Rademacher
  - H randomly sampled columns from Hadamard matrix

Theorem (M,Li, Ballard)

Except with probability at most $\frac{d}{\beta^2}$,

$$\|\mathcal{X} - \widehat{\mathcal{X}}\|_F^2 \leq \left(1 + \frac{\alpha n^{d-1}}{r+p}\right) \sum_{j=1}^{d} \sum_{i=r+1}^{n} \sigma_i^2(X_{(j)})$$

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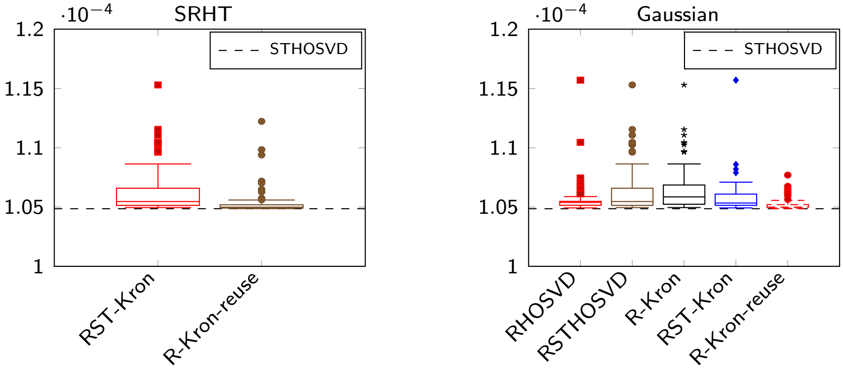
Notes:

- Uses SRHT random matrices that can be represented as a Kronecker product themselves
- Allows for independent product of random matrices per mode, or reuse of same product of random matrices
- Pessimistic compared to accuracy shown in numerical results

Parameters:

- $500 \times 500 \times 500$ tensor with moderately decaying singular values
- target rank $(10, 10, 10)$, oversampling parameter 5, $s = 4$

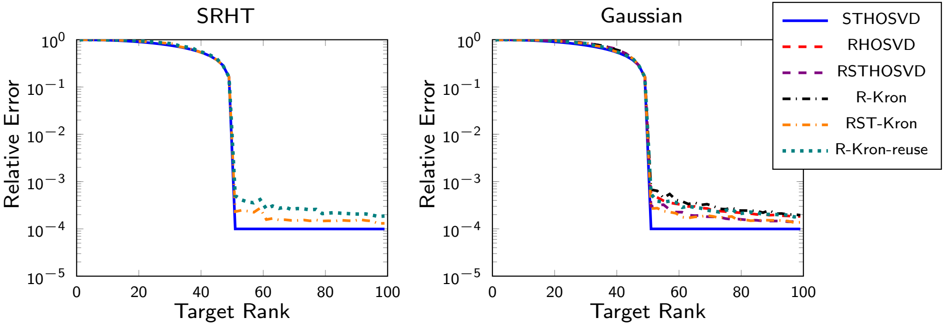
Relative Error over 100 trials



Numerical Results: Accuracy

- $500 \times 500 \times 500$ random tensor with true rank $(50, 50, 50)$ and 10^{-4} noise
- oversampling parameter 5, $s \leq 11$

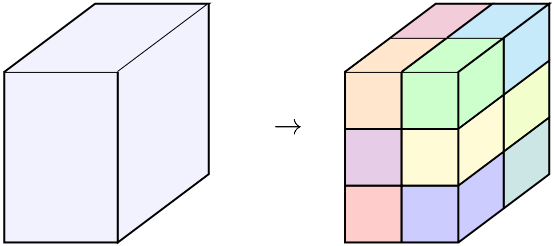
Relative Error with increasing rank



Idea for parallelization

- Store tensor on processor grid
- Parallelize key operations so communication between processors is small as well as cost of computation
- Key operation for our algorithm: multi-TTM

Example: $3 \times 2 \times 2$ processor grid



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All-at-once multi-TTM

Goal: compute $\mathcal{Y} = \mathcal{X} \times_1 U_1 \times_2 U_2 \times \cdots \times_k U_k$ for $k \leq d$ matrices

Two approaches based on communication: in sequence and all-at-once

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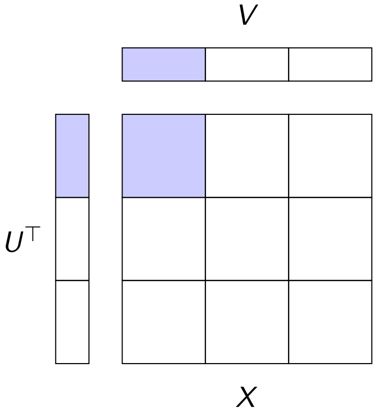

In sequence[1]:

- Compute local $U^\top X$, communicate result
- Compute local multiply with V, communicate result

[1] Ballard, Klinvex, Kolda, ACM TOMS, 2020

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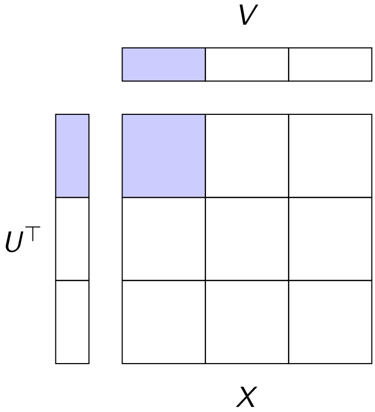

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- Communicates final result

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Comparison: multi-TTM

In-sequence:

- fewer flops, more communication

All-at-once:

- slightly more flops, generally less communication

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Comparison: multi-TTM

In-sequence:

- fewer flops, more communication
- better choice when matrices are fat
- In randomized HOSVD algorithm, use for core multi-TTM $\mathcal{G} = \mathcal{X} \times_1 A_1^\top \times \cdots \times_d A_d^\top$
- factor matrices A_j have more $(r + p)$ columns

All-at-once:

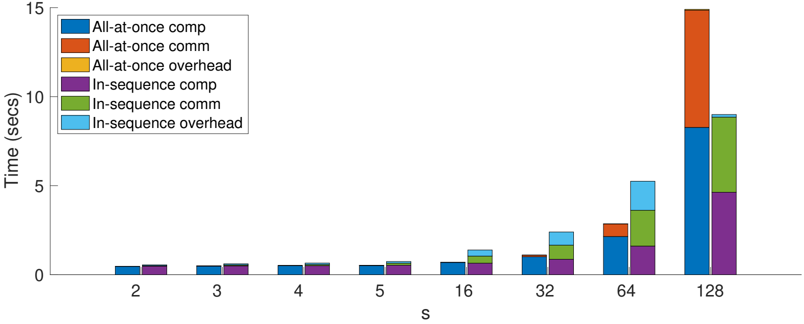
- slightly more flops, generally less communication
- better choice when matrices are skinny
- In randomized HOSVD algorithm, use to compute sketch $\mathcal{Y} = \mathcal{X} \times_2 \Phi_2^\top \times \cdots \times_d \Phi_d^\top$
- random matrices are very skinny (s columns)

Numerical Results: Parallel Runtime

Parameters:

- 4-way tensor, 250 in each mode
- 16 cores on single multicore server
- Gaussian random matrices

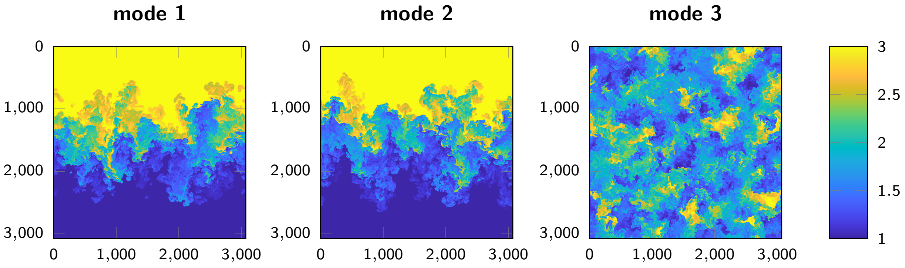
Runtime of multi-TTM methods with increasing number of columns s:



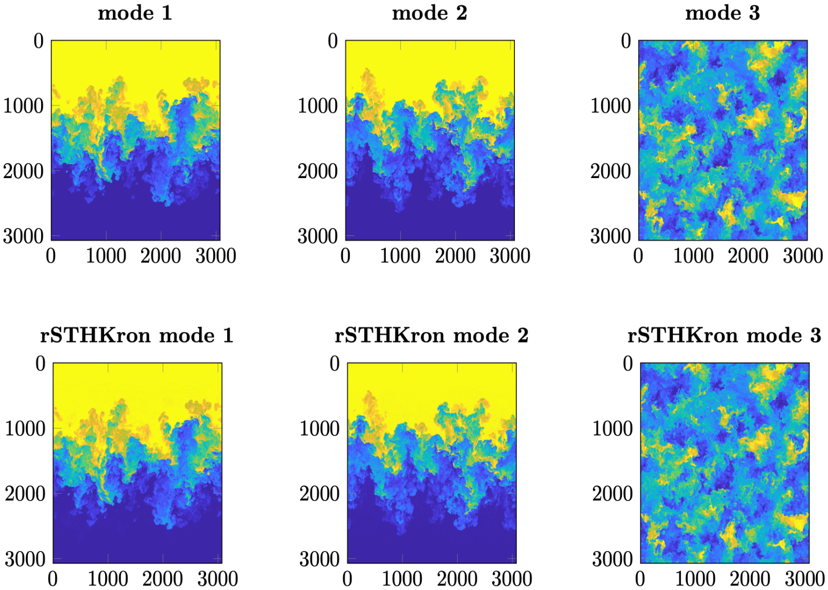
Numerical Results: Miranda Data

Miranda dataset[1]:

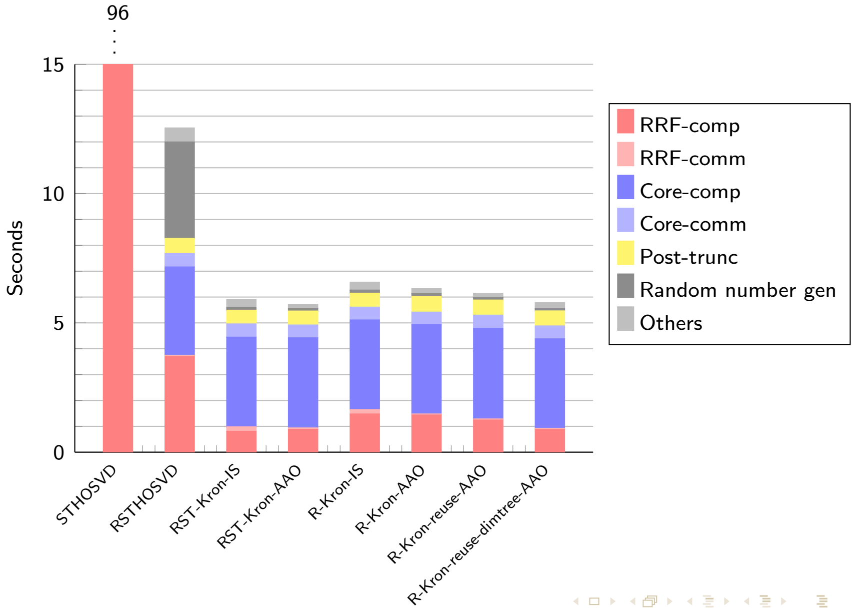
- 3-dimensional simulation data of density ratios, 3072 in each mode
- Target rank $(502, 504, 361) \sim (10^{-2}$ relative error), $s \leq 61$
- On Andes cluster (OLCF)



Numerical Results: Miranda Reconstruction



Numerical Results: Parallel Runtime



Takeaways

Main idea:

Exploiting Kronecker structure and parallelizing key operations of typical randomized HOSVD further reduces the cost of computing Tucker decompositions, and allows for use on distributed systems.

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Exploiting Kronecker structure and parallelizing key operations of typical randomized HOSVD further reduces the cost of computing Tucker decompositions, and allows for use on distributed systems.

Summary:

- Use a Kronecker product of random matrices to use multi-TTM instead of large matrix multiply and reduce number of random entries generated
- Analyze error using new results for Kronecker products of SRHT matrices
- New method for computing a multi-TTM in parallel
  - An all-at-once approach that can communicate less than standard approach and works well with Kronecker product of random matrices in our Tucker algorithms

Minster, Li, Ballard, *Parallel Randomized Tucker Decomposition Algorithms*, arXiv:2211.13028