Parallel Randomized Algorithms for Tucker Decompositions

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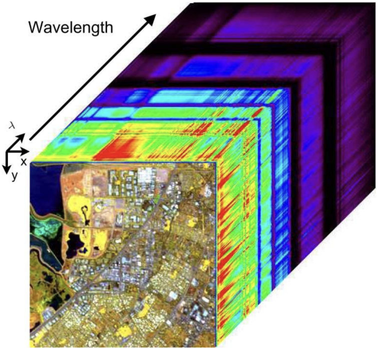
Acknowledgements to NSF CCF 1942892 for funding

Motivation: Multidimensional data

Multidimensional data appears in many applications:

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



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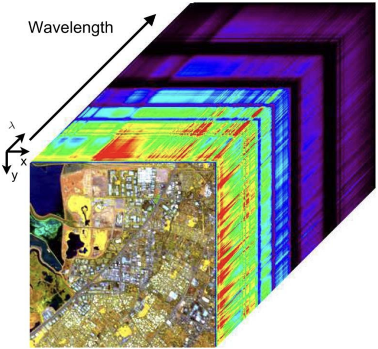

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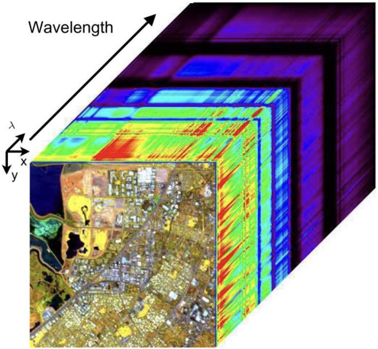

Goal: efficiently obtain compressed representation of data

Method: use parallel, randomized algorithms for Tucker decompositions

- can obtain large compression ratios with high accuracy

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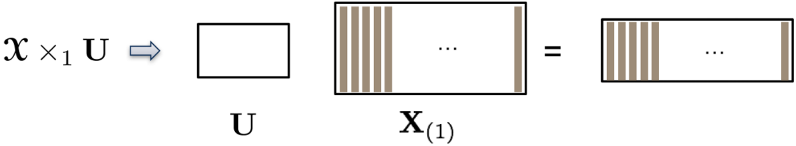
Contributions

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

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

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



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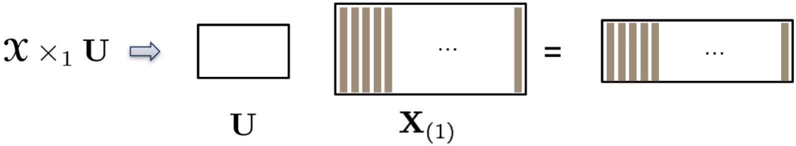


- Multi-TTM: $\mathcal{X} \times_1 U_1 \times_2 U_2 \cdots \times_d U_d$ for d-mode tensor
    - Can be unfolded in j-th mode as

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

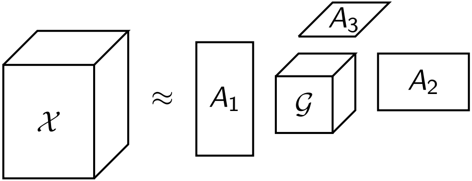
with $\otimes$ the Kronecker product

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]

[1] De Lathauwer, De Moor, Vandewalle, SIAM Journal on Matrix Analysis and Applications, 2000
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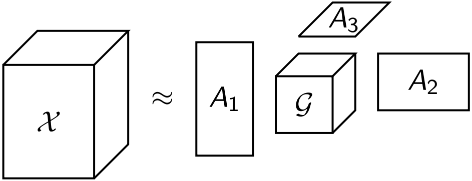

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General approach:

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 $Y = X\Omega$
3. Compute thin QR $Y = QR$

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

Our approach: Kronecker product of random matrices $\Omega = \Phi_1 \otimes \cdots \otimes \Phi_d$ with $\Phi_j \in \mathbb{R}^{n \times s}$, $s^{d-1} = r + p$

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

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Two options for our approach:

1. Use an independent products of Φ_j's per mode

2. Reuse same Kronecker factors Φ_j in Ω_j (i.e., $\Omega_1 = \Phi_2 \otimes \cdots \otimes \Phi_d$)

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Two options for our approach:

1. Use an independent products of Φ_j's per mode
   - Generating and storing more random matrices
   - "rKron"
2. Reuse same Kronecker factors Φ_j in Ω_j (i.e., $\Omega_1 = \Phi_2 \otimes \cdots \otimes \Phi_d$)
   - Allows for reuse of computations
   - Makes analysis more complicated
   - "rKron-reuse"

Theoretical Bound

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-like random matrices: $\Phi = DH$
  - D diagonal Rademacher
  - H randomly sampled columns from Hadamard matrix

Error bound

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

$$\|\mathcal{X} - \widehat{\mathcal{X}}\|_F^2 \leq \left(1 + \frac{\alpha n^{2d-2}}{(r+p)^{d-1}}\right) \|\mathcal{X} - \widehat{\mathcal{X}}_{\text{HOSVD}}\|_F^2$$

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Notes:

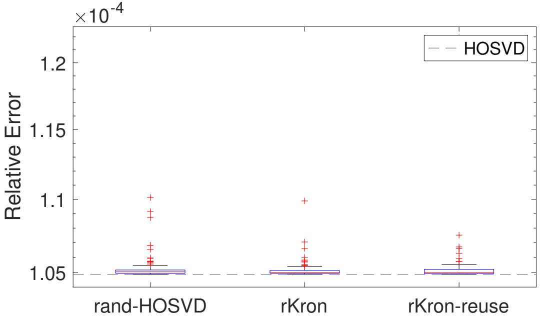
- Pessimistic compared to accuracy shown in numerical results
- Uses SRHT-like random matrices that can be represented as a Kronecker product themselves
- Allows for independent product of random matrices per mode, or reuse of same product of random matrices

Numerical Results: Accuracy

Parameters:

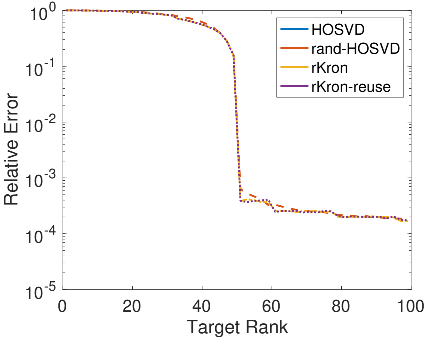
- $500 \times 500 \times 500$ tensor with moderately decaying singular values
- target rank $(10, 10, 10)$, oversampling parameter 5, $s = 4$
- rand-HOSVD: Gaussian random matrix
- rKron, rKron-reuse: SRHT random matrices

Relative Error over 100 trials



- $500 \times 500 \times 500$ random tensor with true rank $(50, 50, 50)$ and 10^{-4} noise
- oversampling parameter 5, $s \leq 11$
- rand-HOSVD: Gaussian random matrix
- rKron, rKron-reuse: SRHT random matrices

Relative Error with increasing rank



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End for

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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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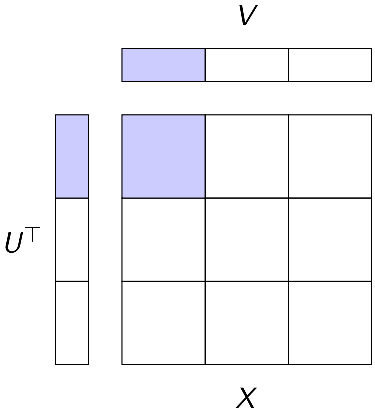
Example: 2 modes $\mathcal{X} \times_1 U^\top \times_2 V^\top = U^\top X V$



In sequence[4]:

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

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

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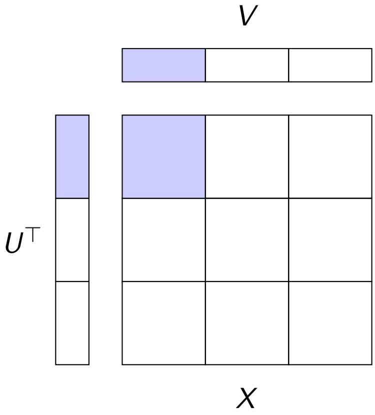

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All-at-once:

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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:

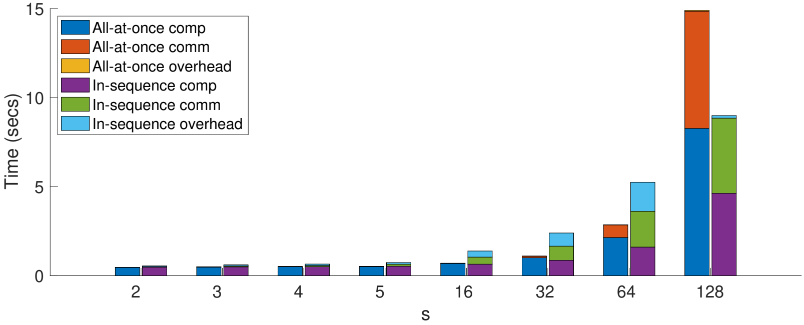
- slightly more flops, generally less communication
- better choice when matrices are skinny
- In randomized HOSVD algorithm, use to compute sketch $\mathcal{Y} = \mathcal{X} \times_2 \Phi_2^\top \times \cdots \times_d \Phi_d^\top$
- random matrices are very skinny (s columns)

Numerical Results: Parallel Runtime

Parameters:

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

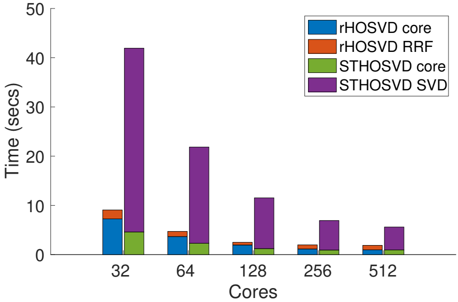
Runtime of multi-TTM methods with increasing number of columns s:



Parameters:

- 4-way tensor, 256 in each mode
- Target rank $(32, 32, 32, 32)$, $s = (3, 3, 4, 4)$
- Gaussian random matrices, rKron-reuse
- On Andes cluster (OLCF)

Runtime of full algorithms with increasing number of cores:



Conclusions

Contributions: new parallel, randomized algorithms for Tucker decompositions

- Use a Kronecker product of random matrices to exploit structure and employ multi-TTM instead of large matrix multiply
- Different versions: re-using or constructing independent Kronecker products
- New method for computing a multi-TTM in parallel
  - An all-at-once approach that can communicate less than standard approach
  - Works well with Kronecker product of random matrices in our Tucker algorithms