FIST-HOSVD: Fused In-place Sequentially Truncated Higher Order Singular Value Decomposition

SIAM PP February 26, 2022

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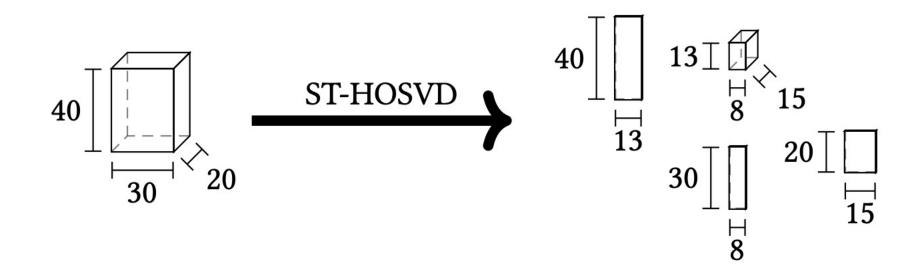
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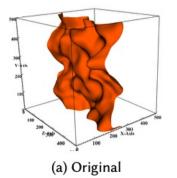


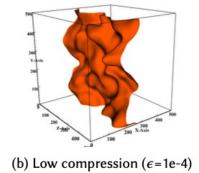
Tucker Decomposition



- Tensor is a multi-dimensional array
- Tucker decomposition compresses tensor
 - Smaller core tensor
 - Set of factor matrices corresponding to each dimension

Applications of Tucker Decomposition





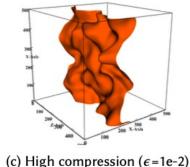
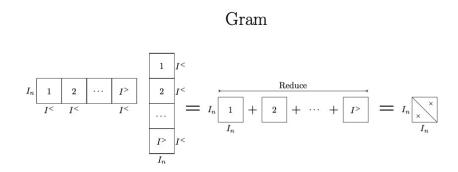


Figure courtesy of:

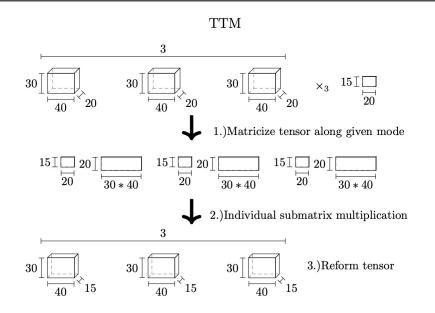
Grey Ballard, Alicia Klinvex, and Tamara G. Kolda. 2020. TuckerMPI: A Parallel C++/MPI Software Package for Large-Scale Data Compression via the Tucker Tensor Decomposition. *ACM Trans. Math. Softw.* 46, 2, Article 13 (June 2020) 31 pages.

- Data Compression
 - TuckerMPI compressed over 6TB of simulation data into 167MB with 1e-2 relative error
 - Can reconstruct entire or part of dataset
 - Error tolerance related to truncation
- Computer Vision
 - TensorFaces, Vasilescu et al.
- Signal Porcessing
 - Lathauwer et al, Muti et al, and more
- And many more...
- Good at capturing latent multi-way relationships between variables
 - Lose information by just viewing as matrix

Computing Tucker via ST-HOSVD

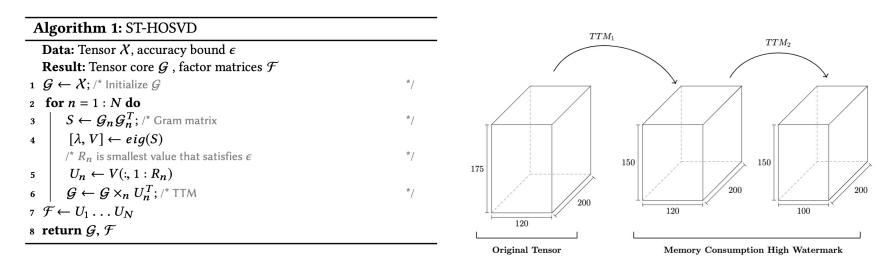


- Two computational bottlenecks
 - Tensor Times Matrix (TTM)
 - Gram
- For tensor *X* with dimensions $I_1 \times \cdots \times I_N$, let:
 - $I_n^* = \prod_{r=1}^N I_r$
 - $I_n^> = \prod_{r=n+1}^N I_r$
 - $I_n^< = \prod_{r=1}^{n-1} I_r$
- mode-*n* TTM with $J \times I_n$ matrix: $O(JI_n^*)$
- Gram along mode- $n: O(I_n I_n^*)$
- Focusing on dense, single-node case



Algorithm 1: ST-HOSVD				
Data: Tensor X , accuracy bound ϵ				
Result: Tensor core ${\mathcal G}$, factor matrices ${\mathcal F}$				
1 $\mathcal{G} \leftarrow \mathcal{X}$; /* Initialize \mathcal{G}	*/			
2 for $n = 1 : N$ do				
$S \leftarrow \mathcal{G}_n \mathcal{G}_n^T; /^* \text{ Gram matrix}$	*/			
$4 \qquad [\lambda, V] \leftarrow eig(S)$				
/* R_n is smallest value that satisfies ϵ	*/			
5 $U_n \leftarrow V(:, 1:R_n)$				
5 $U_n \leftarrow V(:, 1:R_n)$ 6 $\mathcal{G} \leftarrow \mathcal{G} \times_n U_n^T; /^* \text{TTM}$	*/			
7 $\mathcal{F} \leftarrow U_1 \dots U_N$				
8 return \mathcal{G}, \mathcal{F}				

ST-HOSVD Limitations



- In addition to original tensor, must allocate memory to store intermediate TTM results
 - In the worst case when there is little to no truncation, consumes 2x tensor size in memory
- Memory is a limited resource
 - Often bottlenecked by tensor exceeding available memory
- When tensor is larger than $\frac{1}{3}$ main memory (RAM), ST-HOSVD either:
 - Is unable to complete
 - Goes out-of-core → ST-HOSVD thrashes between RAM and Disk, potentially leading to catastrophic performance degradation
- We aim to alleviate this by computing the Tucker decomposition in-place
 - Overwrite the original tensor with core of Tucker decomposition
 - Memory Consumption: $O(I_{max}^2 + \prod_{r=1}^{N} I_r) \rightarrow O(I_{max}^2)$

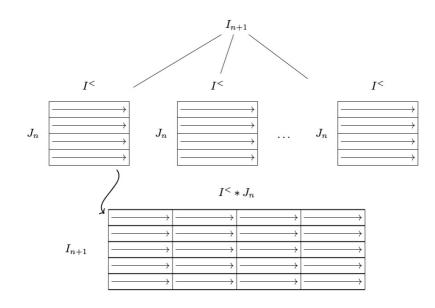
Overview

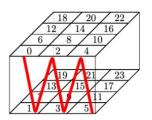
- Memory is a valuable, limited resource
- Significantly decreased memory consumption of computing dense Tucker
 - $O(I_{max}^2 + \prod_{r=1}^N I_r) \to O(I_{max}^2)$
 - If the tensor can be held in memory then we can most likely compute tucker
 - Maintain comparable or decrease runtime

Optimizations

- Develop 3 novel optimizations to efficiently compute Tucker Decomposition in-place:
 - Kernel Fusion
 - Fuse TTM and Gram kernels together to improve memory locality
 - Tensor Tiling
 - Extend matrix tiling and cache blocking to fused kernel operation
 - In-place Transpose
 - Develop blocked in-place transpose algorithm based on cycle-following to prepare cache blocks in-place

Kernel Fusion





	-					
$\left[\begin{array}{rrrr}1&1&1\\2&2&2\end{array}\right]$	×	$\left[\begin{array}{c}0&1\\2&3\\4&5\end{array}\right]\left[$	$\begin{array}{ccc} 6 & 7 \\ 8 & 9 \\ 10 & 11 \end{array}$	$\left]\left[\begin{array}{c} 12\\14\\16\end{array}\right]$	$\begin{bmatrix} 13\\15\\17 \end{bmatrix} \begin{bmatrix} \\ \end{bmatrix}$	$\begin{bmatrix} 18 & 19 \\ 20 & 21 \\ 22 & 23 \end{bmatrix}$
	=	$\left[\begin{array}{c} 6 \\ 12 \\ 12 \\ 18 \end{array}\right] \left[\begin{array}{c} \end{array} \right]$	$\begin{array}{ccc} 24 & 27 \\ 48 & 54 \end{array}$	$\left[\begin{array}{c} 42\\84\end{array}\right]$	$ \begin{array}{c} 45\\90\end{array} $	$\begin{bmatrix} 60 & 63 \\ 20 & 126 \end{bmatrix}$

 $Gram_3$

 TTM_2

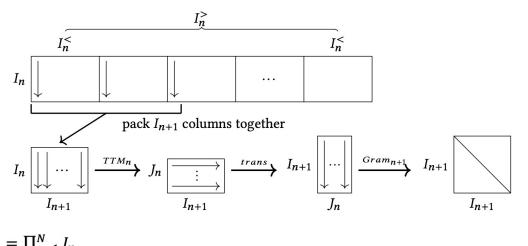
$I_n^r = \prod_{r=1}^n I_r$	-		-	-		-
$I_n^> = \prod_{r=n+1}^N I_r$	$6 \ 9 \ 12 \ 18$			585 193	5 3285 463	5
$n = 117 = n + 1 \cdot 7$	$24 \ 27 \ 48 \ 54$	9 27 45	63	1935 652	5 11115 1570	05
$I_n^{<} = \prod_{r=1}^{n-1} I_r$	42 45 84 90	12 48 84 1	20	3285 1113	$15 \ 18945 \ 2677$	75
n = 11r = 1 r	60 63 120 126	18 54 90 1	.26	4635 1570	05 26775 3784	45

- Compute mode-(n + 1) Gram whilst computing mode-n TTM
 - Fuse TTM and Gram kernels together
- Aim to keep everything in cache

TTM

- Fusing kernels together is known to improve memory locality
 - Especially effective in GPU case \rightarrow future work

Tensor Tiling



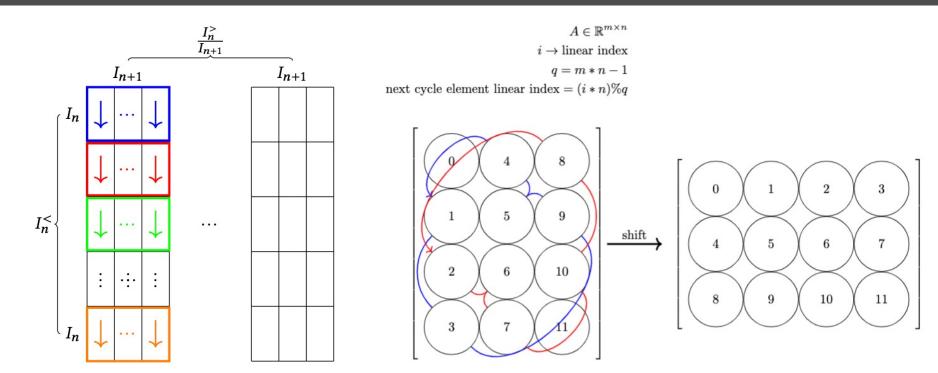
$$I_n^* = \prod_{r=1}^N I_r$$
$$I_n^> = \prod_{r=n+1}^N I_r$$
$$I_n^< = \prod_{r=1}^{n-1} I_r$$

$$n = \prod_{r=n}^{n-1}$$
$$n^{<} = \prod_{r=1}^{n-1}$$

- Pack columns into $I_n \times I_{n+1}$ cache blocks
 - Write $J \times I_{n+1}$ TTM submatrix results in row-major order
 - Then logically transpose to $I_{n+1} \times J$ column-major submatrices
 - No data movement required for logical transpose
- Requires I_{n+1} discontiguous memory accesses on I_n contiguous entries per block
- Tensor layout evolves in memory over course of computation
 - Prepares tensor for subsequent iterations
 - Next dimension contiguous in memory

Algorithm 3: FaST-HOSVD	
Data: Tensor X , accuracy bound ϵ	
Result: Tensor core ${\mathcal G}$, factor matrices ${\mathcal F}$	
/* Initialize ${\cal G}$	*/
1 $\mathcal{G} \leftarrow \mathcal{X}$	
/* First Gram matrix	*/
$2 S_1 \leftarrow \mathcal{G}_1 \mathcal{G}_1^T$	
$[\lambda, V] \leftarrow eig(S_1)$	
4 $U_1 \leftarrow V(:, 1:R_1)$	
/* R_1 is smallest value that satisfies ϵ	*/
5 for $n = 1 : N - 1$ do	
$[\mathcal{G}_{n+1}, \mathcal{S}_{n+1}] \leftarrow Fused_Packed_Kernel(\mathcal{G}_n, U_n, n)$	
7 $[\lambda, V] \leftarrow eig(S_{n+1})$	
8 $U_{n+1} \leftarrow V(:, 1:R_{n+1})$	
/* Last TTM	*/
9 $\mathcal{G} \leftarrow \mathcal{G} \times_n U_N^T$	
10 $\mathcal{F} \leftarrow U_1 \dots U_N$	
11 return \mathcal{G}, \mathcal{F}	

In-place Transpose



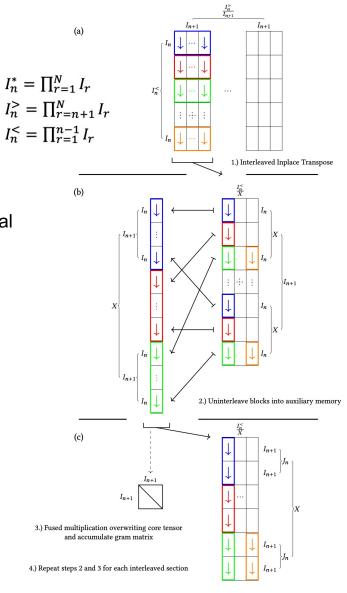
- $I_n^* = \prod_{r=1}^N I_r$ $I_n^> = \prod_{r=n+1}^N I_r$ $I_n^< = \prod_{r=1}^{n-1} I_r$
 - Traditional Cycle-Following based In-place Transpose algorithm
 - Requires less element access than other in-place transpose algorithms
 - In practice suffers from poor memory locality due to almost pseudo-random element access
- Developed blocked variant that improves memory locality, referred to as Interleaved In-Place Transpose (IIPT)
- Plan to compare performance against existing in-place transpose algorithms in future work

FIST-HOSVD

- Interleaved In-place Transpose to prepare cache blocks
- Copy cache blocks into auxiliary memory allocation
 - deinterleave cache blocks during copy
- Perform fused multiplication on each cache block
 - Result overwrites corresponding section of tensor
- Avoids allocating memory to hold intermediate TTM results
- If the tensor can be held in memory with at least $O(I_{max}^2)$ additional elements worth of memory, then we can compute Tucker

Algorithm 6: FIST-HOSVD

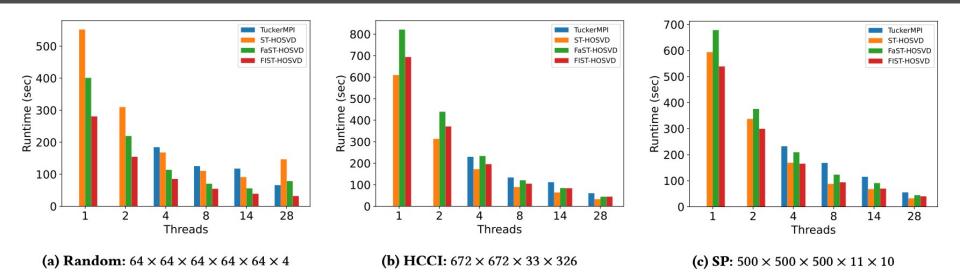
Data: Tensor X, auxiliary memory limit in β **Result:** X overwritten with core tensor. Factor matrices \mathcal{F} 1 $S_0 \leftarrow X_1 X_1^T$; /* First Gram matrix */ 2 for n = 1 : N - 1 do $[\lambda, V] \leftarrow eig(S_n)$ 3 $U_n \leftarrow V(:, 1: R_n); /* R_n$, smallest value that satisfies ϵ */ 4 $S_{n+1} \leftarrow \text{Fused_Inplace_kernel}(\mathcal{G}, U_n, \beta)$ 5 6 $[\lambda, V] \leftarrow eig(S_N)$ 7 $U_N \leftarrow V(:, 1:R_N)$ 8 $X \leftarrow X \times_N U_N^T$; /* Last Inplace TTM */ 9 $\mathcal{F} \leftarrow U_1 \ldots U_N$ 10 return \mathcal{F}



Experimental set-up

- Each node has 28 cores and 256GB memory
 - Allocating more than this allocation either causes the program to terminate or the node to crash
- Three different datasets:
 - Randomly generated
 - Used to represent high-rank tensor
 - Each timeslice is: 64×64×64×64×64
 - Homogeneous Charge Compression Ignition (HCCI)
 - 4-th order tensor from a simulation of turbulent autoignition over a 2D spatial domain
 - Each timeslice is: 672×672×33
 - Statistically Planar (SP)
 - 5-th order tensor from a simulation over a 3D spatial domain, 4-th mode is 11 solution variables at each grid point
 - Each timeslice is: 500×500×500×11

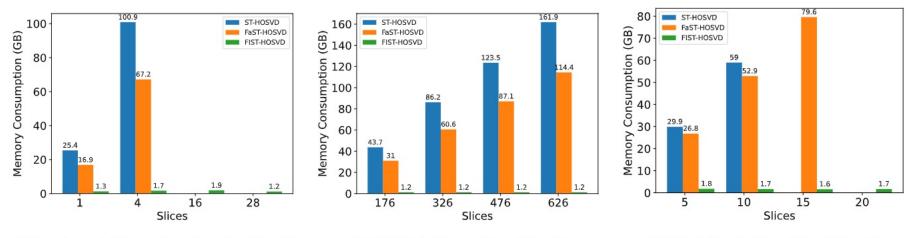
Runtime Results



Sample bar charts of runs with an error-tolerance (ϵ) of 1e-07. Bars not shown did not complete due to running out of memory.

- Fused implementations performs better along later dimensions due to cache blocking
- Cache blocking incurs data movement overhead
- Plan to add support for processing dimensions out of order in future work
- Maintain comparable runtime

Memory Consumption



(a) Random: 1 slice is $64 \times 64 \times 64 \times 64 \times 64$

(b) HCCI: 1 slice is 672 × 672 × 33

(c) SP: 1 slice is 500 × 500 × 500 × 11

Memory consumption over different timeslice counts for an error-tolerance (ϵ) of 1e-07. Bars not shown did not complete due to running out of memory.

FIST-HOSVD consumes significantly less memory than the other algorithms

$$\mathcal{O}(I_{max}^2 + \prod_{r=1}^N I_r) \rightarrow \mathcal{O}(I_{max}^2)$$

- Compute memory consumption as: memory highwater mark of program size of orignal tensor
- Allocated 1GB of auxiliary memory for FIST-HOSVD
 - Additional memory usage comes from Gram reduction

Summary

- Recap:
 - Memory Consumption: $O(I_{max}^2 + \prod_{r=1}^{N} I_r) \rightarrow O(I_{max}^2)$
 - Significantly decreased memory consumption of ST-HOSVD for dense Tucker
 - If tensor fits in memory, then FIST-HOSVD can most likely compute Tucker
 - Maintained comparable or decreased runtime
- Future Work:
 - Add in support for processing dimensions in any order
 - Kernel fusion provides biggest performance improvements along later dimensions
 - Compare IIPT algorithm to other in-place transpose algorithms
 - Complete GPU port
 - Everything implemented in Kokkos (portable framework)
 - Kernel fusion originally intended for GPU case
 - Device memory even more limited than host memory



Questions?

Backup Slides

Runtime Tables

Table 1: Random tensor runtime (in seconds).

1 slice: $64 \times 64 \times 64 \times 64 \times 64$

ϵ	Slices:	1	4	16	28
	TuckerMPI	13.4	66.5	_	-
1 - 00	ST-HOSVD	4.4	142.1	—	-
1e-09	FaST-HOSVD	4.4	70.0	_	-
	FIST-HOSVD	5.5	32.3	107.6	219.3
	TuckerMPI	13.4	66.4	_	-
1e-05	ST-HOSVD	4.4	143.8	_	-
16-05	FaST-HOSVD	4.3	74.8	—	-
	FIST-HOSVD	5.5	32.1	107.3	219.8
	TuckerMPI	13.5	65.6	_	-
1e-03	ST-HOSVD	4.4	143.3	—	-
1e-05	FaST-HOSVD	4.4	70.8	_	-
	FIST-HOSVD	5.6	32.7	107.4	219.6

Table 2: HCCI tensor runtime (in seconds).1 slice: $672 \times 672 \times 33$

Table 3: SP tensor runtime (in seconds).1 slice: $500 \times 500 \times 500 \times 11$

ϵ	Slices:	176	326	476	626		ϵ
	TuckerMPI	35.4	71.4	104.9	_		
1e-09	ST-HOSVD	18.0	37.4	58.6	_		
16-09	FaST-HOSVD	23.9	47.8	76.0	125.2		1e-0
	FIST-HOSVD	25.0	51.2	77.6	105.7		
1e-05	TuckerMPI	20.0	43.7	63.8	84.2		1e-0
	ST-HOSVD	9.6	23.3	35.6	47.7		
	FaST-HOSVD	12.0	31.3	44.8	66.7		
	FIST-HOSVD	13.5	31.5	45.7	60.2		
	TuckerMPI	11.4	27.1	38.3	49.1		
1e-03	ST-HOSVD	5.7	12.6	19.5	25.6		1.0
	FaST-HOSVD	6.9	16.0	24.3	33.5		1e-0
	FIST-HOSVD	7.0	16.5	24.7	31.6		

ϵ	Slices:	5	10	15	20
	TuckerMPI	34.0	-	_	—
1- 00	ST-HOSVD	24.9	38.6	-	-
1e-09	FaST-HOSVD	35.1	54.2	—	-
	FIST-HOSVD	25.6	49.3	72.7	92.6
	TuckerMPI	12.9	25.4	38.1	-
1e-05	ST-HOSVD	10.1	19.2	28.9	-
16-05	FaST-HOSVD	12.2	22.8	35.5	_
	FIST-HOSVD	12.5	24.3	36.4	48.2
	TuckerMPI	8.4	16.6	24.8	33.3
1e-03	ST-HOSVD	7.0	13.9	21.36	27.6
16-05	FaST-HOSVD	9.5	18.9	29.0	37.9
	FIST-HOSVD	9.9	19.4	28.9	38.4

ϵ	Dataset	Slices	Resulting Core
	Random	4	$64 \times 64 \times 64 \times 64 \times 64 \times 4$
1e-09	HCCI	326	$631 \times 610 \times 31 \times 326$
	SP *	20	$187 \times 288 \times 278 \times 9 \times 20$
	Random	4	$64 \times 64 \times 64 \times 64 \times 64 \times 4$
1e-05	HCCI	326	$433 \times 410 \times 33 \times 234$
	SP *	20	$79 \times 116 \times 117 \times 7 \times 5$
	Random	4	$64 \times 64 \times 64 \times 64 \times 64 \times 4$
1e-03	HCCI	326	$232\times217\times29\times81$
	SP	20	$27 \times 48 \times 48 \times 2 \times 3$

Memory Consumption Tables

Table 5: Random tensor memory consumption (in GB). Table 1 slice is ~ 8 GB

Slices: 1 4 16 28 ϵ ST-HOSVD 24.296.2 _ _ 1e-09 FaST-HOSVD 16.2 64.1 _ _ FIST-HOSVD 1.2 1.6 1.9 1.2 ST-HOSVD 96.2 24.2_ _ FaST-HOSVD 1e-05 16.264.1 _ _ FIST-HOSVD 1.2 1.6 1.9 1.2 96.2 24.2 ST-HOSVD _ _ FaST-HOSVD 1e-03 16.2 64.1 _ _ FIST-HOSVD 1.2 1.6 1.9 1.2

ble 6: HCCI tensor memory consumption (in GB).
1 slice is ~ 0.12 GB

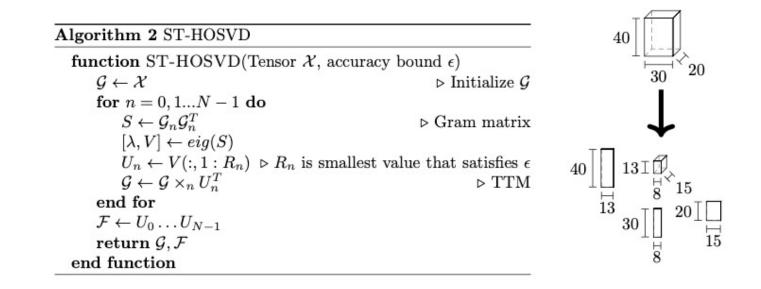
e	Slices:	176	326	476	626
	ST-HOSVD	49.0	94.0	135.6	_
1e-09	FaST-HOSVD	34.2	65.2	94.1	123.0
	FIST-HOSVD	1.1	1.1	1.1	1.1
	ST-HOSVD	18.4	47.3	65.8	82.5
1e-05	FaST-HOSVD	15.2	37.9	54.1	70.1
	FIST-HOSVD	1.1	1.2	1.1	1.1
	ST-HOSVD	6.7	17.7	24.1	30.6
1e-03	FaST-HOSVD	6.8	17.0	23.4	29.8
	FIST-HOSVD	1.1	1.2	1.3	1.3

Table 7: SP tensor memory consumption (in GB). 1 slice is $\sim 11~\text{GB}$

ε	Slices:	5	10	15	20
	ST-HOSVD	35.5	70.3	_	-
1e-09	FaST-HOSVD	30.8	60.2	-	-
	FIST-HOSVD	1.5	1.8	1.5	1.7
	ST-HOSVD	10.4	20.4	30.4	_
1e-05	FaST-HOSVD	10.3	20.2	30.2	-
	FIST-HOSVD	1.2	1.2	1.4	1.3
	ST-HOSVD	3.2	6.3	9.3	12.3
1e-03	FaST-HOSVD	3.3	6.3	9.4	12.4
	FIST-HOSVD	1.1	1.1	1.1	1.1

ϵ	Dataset	Slices	Resulting Core
	Random	4	$64 \times 64 \times 64 \times 64 \times 64 \times 4$
1e-09	HCCI	326	$631 \times 610 \times 31 \times 326$
	SP *	20	$187 \times 288 \times 278 \times 9 \times 20$
	Random	4	$64 \times 64 \times 64 \times 64 \times 64 \times 4$
1e-05	HCCI	326	$433 \times 410 \times 33 \times 234$
	SP *	20	$79 \times 116 \times 117 \times 7 \times 5$
	Random	4	$64 \times 64 \times 64 \times 64 \times 64 \times 4$
1e-03	HCCI	326	$232\times217\times29\times81$
	SP	20	$27 \times 48 \times 48 \times 2 \times 3$

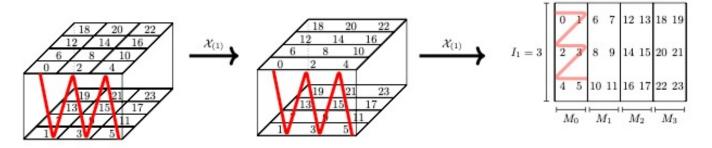
How to compute Tucker



- Several algorithms
 - HOOI, HOSVD, T-HOSVD, ST-HOSVD etc
- Sequentially Truncated Higher Order Singular Value Decomposition
 - ST-HOSVD
 - Truncates tensor at each iteration to save on FLOPs
 - Arguably fastest and most common method to compute Tucker

Helpful Notation

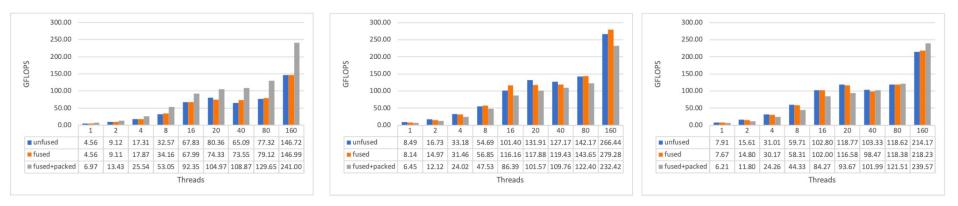
- X is a tensor of order N with dimension sizes: I₁× ... I_N
 Assume starts stored in column major order
- Mode *n* fibers: set of vectors resulting from holding the *n*th mode constant and iterating over all other dimensions
- Mode n matricization: matrix whose columns are the mode – n tensor fibers of X, denoted X_(n)
- Useful values: $I_n^> = \prod_{r=n+1}^N I_r$, $I_n^< = \prod_{r=1}^{n-1} I_r$



ST-HOSVD Bottlenecks

- Two kernels: TTM and Gram
- Tensor Times Matrix (TTM)
 - Can be viewed as batched matrix multiplication
 - Multiplies tensor along n^{th} dimension by $R_n \times I_n$ matrix
 - Input tensor dimensions are: $I_1 \times ... I_n ... \times I_N$
 - Output tensor dimensions are: $I_1 \times ... R_n ... \times I_N$
- Gram
 - Matricized tensor multiplied by its transpose
 - $I_n \times (I_1 * \dots I_{n-1} * I_{n+1} \dots * I_N) * I_n \times (I_1 * \dots I_{n-1} * I_{n+1} \dots * I_N)^T$
 - Result is: symmetric $I_n \times I_n$ matrix
- Depending on size of R_n relative to I_n , require asymptotically comparable amounts of work

Benchmark results



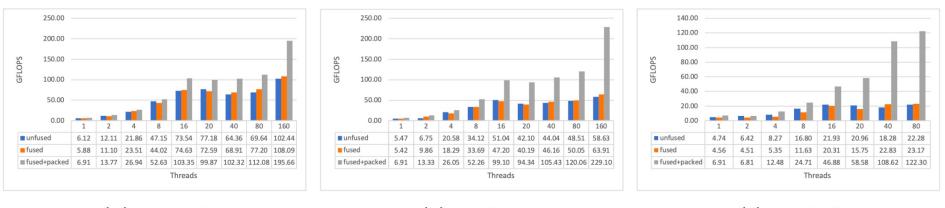
(a) mode-0

(b) mode-1

(c) mode-2

- 16×16×16×16×16×16
 - Dense, random tensor
- Uses KokkosKernel's SerialGemm
- Run on IBM Power 9
- Comparison of:
 - Unfused TTM + Gram
 - Fused
 - Fused+packed

Another page of graphs



(d) mode-3

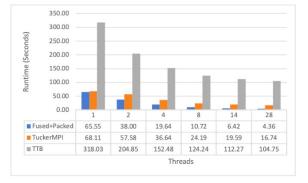
(e) mode-4

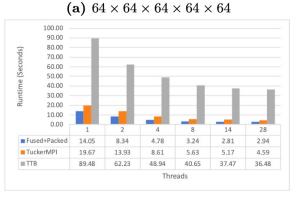
(f) mode-5

- Later modes submatrices become very long
 - Start falling out of cache
 - Begin to require skinny matrix multiplications that many GEMM kernels are not optimized for
- Packed blocks maintain performance for later dimensions
- Well worth the packing overhead

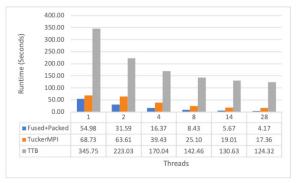
Benchmark results (cont.)

- 4 dense, random tensors
 - Error tolerance = 0
- All use MKL
- Run on Intel Xeon E5
 - 14 cores per socket
 - 2 sockets
- Comparison of:
 - Proposed Fused+Packed
 - TuckerMPI
 - Matlab Tensor Toolbox
- Fused+Packed scales better

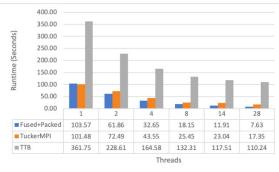




(c) $16 \times 16 \times 16 \times 16 \times 16 \times 16 \times 16$



(b) $32 \times 32 \times 32 \times 32 \times 32 \times 32$



(d) $4 \times 128 \times 128 \times 128 \times 128$

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