Communication-Optimal Algorithms for CP Decompositions of Dense Tensors

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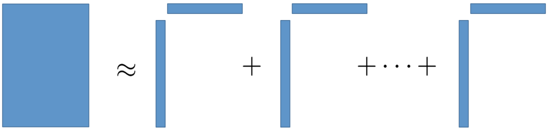
Summary

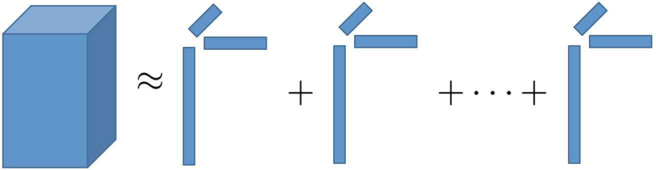
- We establish communication lower bounds for matricized-tensor times Khatri-Rao product (MTTKRP)
  - key kernel for computing CP decomposition
- We present optimal parallel dense MTTKRP algorithm
  - attains the lower bound to within constant factors
- We implement and benchmark optimal CP-ALS algorithm
  - remains computation bound and scales well
  - dimension tree optimization avoids redundant computation

CP Decomposition: sum of outer products

Matrix: $$\mathbf{M} \approx \sum_{r=1}^{R} \mathbf{u}_r(\sigma_r \mathbf{v}_r^T)$$

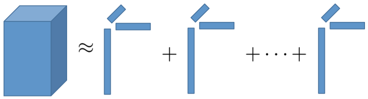


Tensor: $$\mathcal{X} \approx \sum_{r=1}^{R} \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r$$



This is known as the CANDECOMP or PARAFAC or canonical polyadic or CP decomposition

CP Optimization Problem



For fixed rank R, we want to solve

$$\min_{\mathbf{U},\mathbf{V},\mathbf{W}} \left\| \mathcal{X} - \sum_{r=1}^{R} \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r \right\|$$

which is a nonlinear, nonconvex optimization problem

- in the matrix case, the SVD gives us the optimal solution
- in the tensor case, need iterative optimization scheme

Alternating Least Squares (ALS)

Fixing all but one factor matrix, we have a linear LS problem:

$$\min_{\mathbf{V}} \left\| \mathcal{X} - \sum_{r=1}^{R} \hat{\mathbf{u}}_r \circ \mathbf{v}_r \circ \hat{\mathbf{w}}_r \right\|$$

or equivalently

$$\min_{\mathbf{V}} \left\| \mathbf{X}_{(2)} - \mathbf{V}(\hat{\mathbf{W}} \odot \hat{\mathbf{U}})^{\mathsf{T}} \right\|_F$$

$\odot$ is the Khatri-Rao product, a column-wise Kronecker product or row-wise Hadamard (element-wise) product

ALS works by alternating over factor matrices, updating one at a time by solving the corresponding linear LS problem

CP-ALS

Repeat

1. Solve $\mathbf{U}(\mathbf{V}^\mathsf{T}\mathbf{V} * \mathbf{W}^\mathsf{T}\mathbf{W}) = \mathbf{X}_{(1)}(\mathbf{W} \odot \mathbf{V})$ for $\mathbf{U}$
2. Solve $\mathbf{V}(\mathbf{U}^\mathsf{T}\mathbf{U} * \mathbf{W}^\mathsf{T}\mathbf{W}) = \mathbf{X}_{(2)}(\mathbf{W} \odot \mathbf{U})$ for $\mathbf{V}$
3. Solve $\mathbf{W}(\mathbf{U}^\mathsf{T}\mathbf{U} * \mathbf{V}^\mathsf{T}\mathbf{V}) = \mathbf{X}_{(3)}(\mathbf{V} \odot \mathbf{U})$ for $\mathbf{W}$

Linear least squares problems solved via normal equations using identity $(\mathbf{A} \odot \mathbf{B})^\mathsf{T}(\mathbf{A} \odot \mathbf{B}) = \mathbf{A}^\mathsf{T}\mathbf{A} * \mathbf{B}^\mathsf{T}\mathbf{B}$, where $*$ is Hadamard product

All optimization schemes that compute the gradient must also compute MTTKRP in all modes: e.g.,

$$\frac{\partial f}{\partial \mathbf{V}} = \mathbf{V}(\mathbf{U}^\mathsf{T}\mathbf{U} * \mathbf{W}^\mathsf{T}\mathbf{W}) - \mathbf{X}_{(2)}(\mathbf{W} \odot \mathbf{U})$$

MTTKRP bottleneck

- How do we compute MTTKRP efficiently?

- How do we parallelize MTTKRP efficiently?
  - how do we load balance computation?
  - how do we minimize communication?

MTTKRP via Matrix Multiplication

MTTKRP: $\mathbf{M} = \mathbf{X}_{(2)}(\mathbf{W} \odot \mathbf{U})$

Standard approach to MTTKRP for dense tensors

1. "form" matricized tensor (a matrix)
2. compute Khatri-Rao product (a matrix)
3. call matrix-matrix multiplication subroutine

Can we communicate less by exploiting tensor structure?
(avoiding forming explicit Khatri-Rao product)

MTTKRP for 3-way Tensors

Matrix equation:

$$\mathbf{M} = \mathbf{X}_{(2)}(\mathbf{W} \odot \mathbf{U})$$

Element equation:

$$m_{jr} = \sum_{i=1}^{I} \sum_{k=1}^{K} x_{ijk} u_{ir} w_{kr}$$

Example pseudocode:

for $i = 1$ to I **do**
  for $j = 1$ to J **do**
    for $k = 1$ to K **do**
      for $r = 1$ to R **do**
        $\mathbf{M}(j, r) \mathrel{+}= \mathcal{X}(i, j, k) \cdot \mathbf{U}(i, r) \cdot \mathbf{W}(k, r)$

MTTKRP for N-way Tensors

Matrix equation:

$$\mathbf{M}^{(n)} = \mathbf{X}_{(n)}(\mathbf{U}^{(N)} \odot \cdots \odot \mathbf{U}^{(n+1)} \odot \mathbf{U}^{(n-1)} \odot \cdots \odot \mathbf{U}^{(1)})$$

Element equation:

$$m^{(n)}_{i_n r} = \sum x_{i_1 \dots i_N} \prod_{m \neq n} u^{(m)}_{i_m r}$$

Example pseudocode:

for $i_1 = 1$ to I_1 **do**

$\ddots$

for $i_N = 1$ to I_N **do**

for $r = 1$ to R **do**

$\mathbf{M}^{(n)}(i_n, r) \mathrel{+}= \mathcal{X}(i_1, \dots, i_N) \cdot \mathbf{U}^{(1)}(i_1, r) \cdots \mathbf{U}^{(N)}(i_N, r)$

Communication Lower Bounds for MTTKRP

MTTKRP is a set of nested loops that accesses arrays

- Nick's PhD thesis was "Communication-Optimal Loop Nests"
- References: thesis [Kni15] and paper [CDK$^+$13]

From Nick's thesis...

- tabulate how the arrays are accessed
- use Hölder-Brascamp-Lieb-type inequality in LB proof
- solve linear program to get tightest lower bound

MTTKRP Lower Bound Proofs

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- Gotcha: memory-independent bounds most relevant
  - inspiration from matrix multiplication [BDH+12, DEF+13]

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- Gotcha: memory-independent bounds most relevant
  - inspiration from matrix multiplication [BDH$^+$12, DEF$^+$13]
- Key assumption: algorithm is not allowed to pre-compute and re-use temporary values
  - e.g., forming explicit Khatri-Rao product
  - e.g., computing and re-using “partial” MTTKRP

Parallel Communication Lower Bound

Theorem

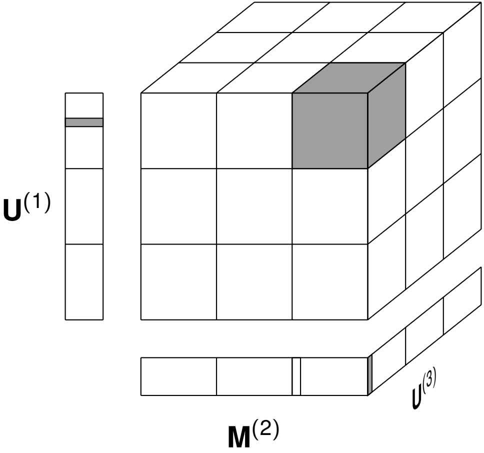
Any parallel MTTKRP algorithm involving a tensor with $I_k = I^{1/N}$ for all k and that evenly distributes one copy of the input and output performs at least

$$\Omega\left(\left(\frac{NIR}{P}\right)^{\frac{N}{2N-1}} + NR\left(\frac{I}{P}\right)^{1/N}\right)$$

sends and receives. (Either term can dominate.)

- N is the number of modes
- I is the number of tensor entries
- I_k is the dimension of the kth mode
- R is the rank of the CP model
- P is the number of processors

Communication-Optimal Parallel Algorithm (3D)



Each processor

1. Starts with one subtensor and subset of rows of each input factor matrix

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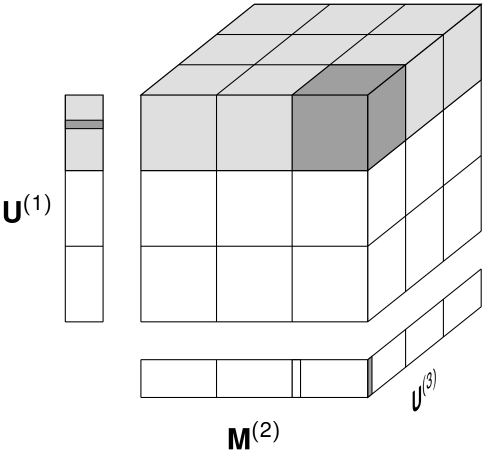

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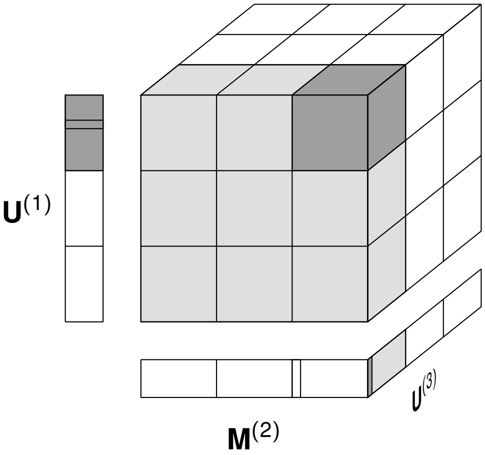

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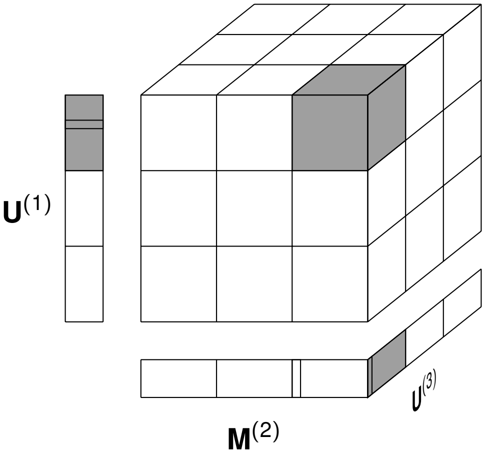

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4. Computes its contribution to rows of $\mathbf{M}^{(2)}$ (local MTTKRP)

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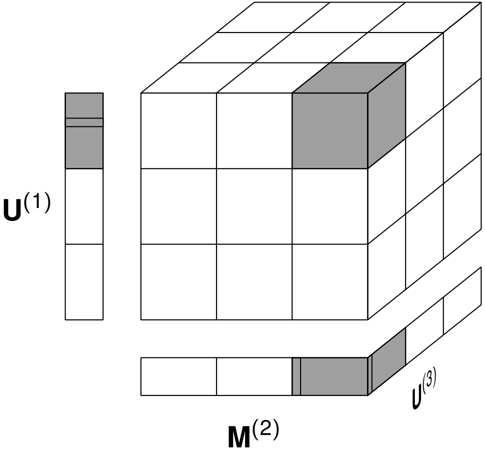

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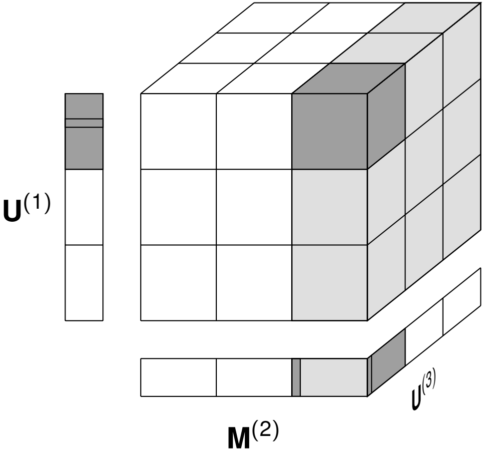

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5. Reduce-Scatters to compute and distribute $\mathbf{M}^{(2)}$ evenly

Theoretical Comparisons

	Lower Bound	New Algorithm	Standard (MM*)
Words ("small" P)	$\Omega\left(NR\left(\frac{I}{P}\right)^{1/N}\right)$	$O\left(NR\left(\frac{I}{P}\right)^{1/N}\right)$	$O\left(I^{1/N}R\right)$

- For relatively small P (or small R) and even dimensions, parallel "stationary" algorithm attains lower bound
  - same algorithm for sparse [SK16] and dense 3D [LKL$^+$17]

Theoretical Comparisons

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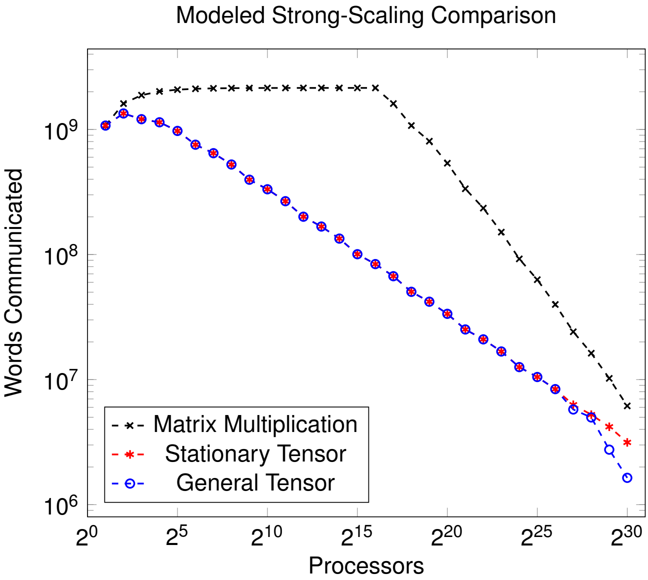
Words ("large" P)	$\Omega\left(\left(\frac{NIR}{P}\right)^{\frac{N}{2N-1}}\right)$	$O\left(\left(\frac{NIR}{P}\right)^{\frac{N}{2N-1}}\right)$	$O\left(\left(\frac{IR}{P}\right)^{2/3}\right)$

- For relatively small P (or small R) and even dimensions, parallel "stationary" algorithm attains lower bound
  - same algorithm for sparse [SK16] and dense 3D [LKL$^+$17]
- For larger P (or R), then we need more general algorithm to attain lower bound
  - involves communicating the tensor

*communication-optimal matrix multiplication from [DEF$^+$13]

Modeled Communication Costs



What about for a full CP-ALS iteration?

A full iteration of CP-ALS includes computing all N MTTKRPs

Lower Bound
Lower bound for single MTTKRP applies to computing all N

Algorithm
We can compute all N with same communication as just 1

- lots of data overlap across MTTKRPs
- more computation required, but not that much more

Avoiding re-communication across MTTKRPs

while not converged **do**
  for $n = 1$ to N **do**
    % *Compute new factor matrix in nth mode*
    $\mathbf{M} = \text{Local-MTTKRP}(\mathcal{X}_{p_1 \cdots p_N}, \{\mathbf{U}_{p_i}^{(i)}\}, n)$
    $\mathbf{M}_{\mathbf{p}}^{(n)} = \text{Reduce-Scatter}(\mathbf{M}, \textsc{Proc-Slice}(n, p_n))$
    $\mathbf{S}^{(n)} = \mathbf{G}^{(1)} * \cdots * \mathbf{G}^{(n-1)} * \mathbf{G}^{(n+1)} * \cdots * \mathbf{G}^{(N)}$
    $\mathbf{U}_{\mathbf{p}}^{(n)} = \text{Local-Update}(\mathbf{S}^{(n)}, \mathbf{M}_{\mathbf{p}}^{(n)})$
    % *Organize data for later modes*
    $\mathbf{H} = \mathbf{U}_{\mathbf{p}}^{(n)\mathsf{T}} \mathbf{U}_{\mathbf{p}}^{(n)}$
    $\mathbf{G}^{(n)} = \text{All-Reduce}(\mathbf{H}, \textsc{All-Procs})$
    $\mathbf{U}_{p_n}^{(n)} = \text{All-Gather}(\mathbf{U}_{\mathbf{p}}^{(n)}, \textsc{Proc-Slice}(n, p_n))$

Compute factor matrix, communicate it **once** for use in all other $N-1$ modes

Avoiding recomputation across MTTKRPs

We re-use communication and computation across MTTKRPs

$$\mathbf{M}^{(1)} = \underline{\mathbf{X}_{(1)} \left(\mathbf{U}^{(3)}\right.} \odot \left.\mathbf{U}^{(2)}\right) \qquad \text{and} \qquad \mathbf{M}^{(2)} = \underline{\mathbf{X}_{(2)} \left(\mathbf{U}^{(3)}\right.} \odot \left.\mathbf{U}^{(1)}\right)$$

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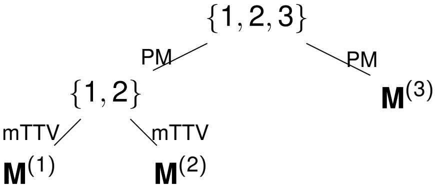
We organize intermediate values in "dimension tree" [PTC13, LCP$^+$17, KU18]



PM = Partial MTTKRP   mTTV = multi-Tensor-Times-Vector

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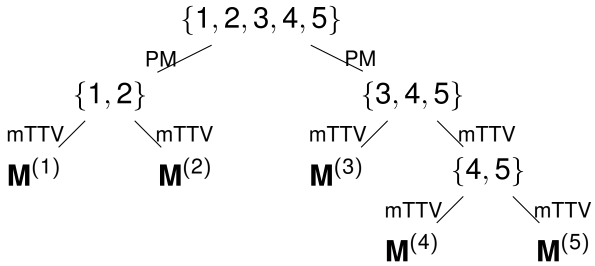

PM = Partial MTTKRP   mTTV = multi-Tensor-Times-Vector

Implementation

- Uses CP-ALS for non-negative CP problems
  - minimize least squares loss function
  - use block principal pivoting [KP11] to solve subproblems
- Avoids redundant communication across MTTKRPs
- Avoids redundant computation across MTTKRPs using dimension trees

Strong Scaling Results (3D)

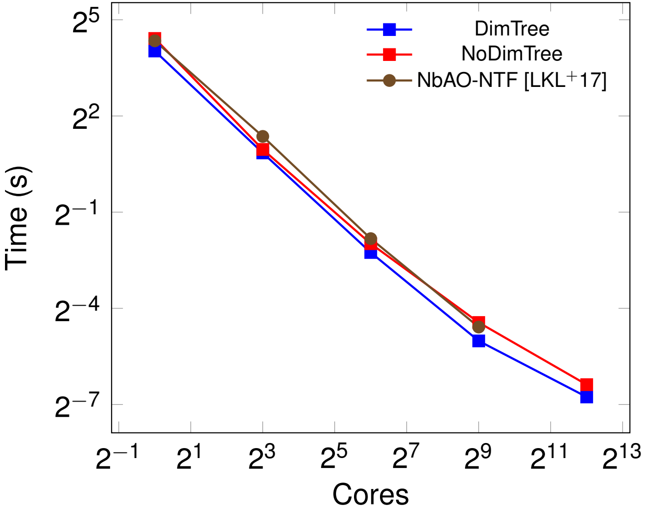

Figure: $1024 \times 1024 \times 1024$ tensor on $2^k \times 2^k \times 2^k$ proc grids ($R = 32$)

Strong Scaling Results (5D)

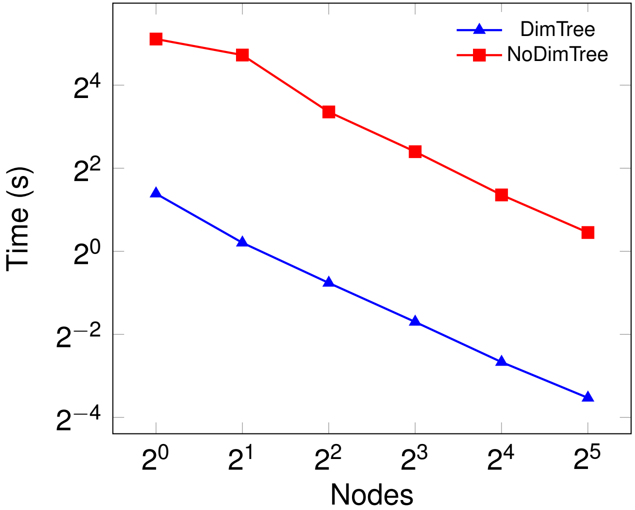

Figure: $64 \times 64 \times 64 \times 64 \times 64$ tensor ($R = 32$)

Varying Rank Results (3D)

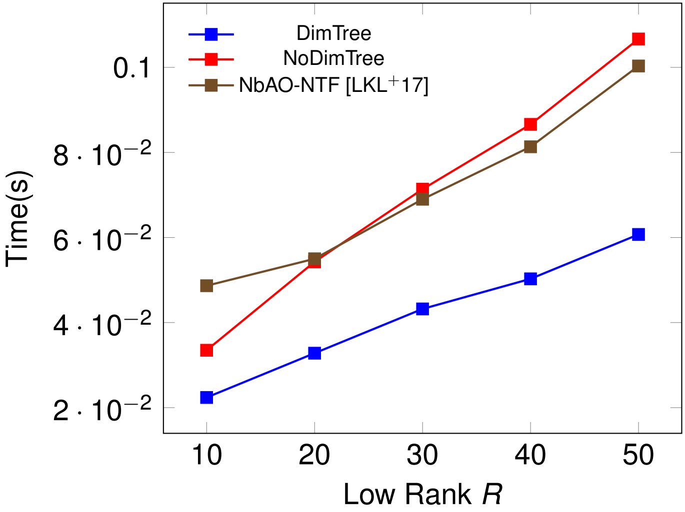

Figure: 30,012 × 1200 × 500 tensor on 120 × 6 × 2 proc grid

Varying Rank Results (4D)

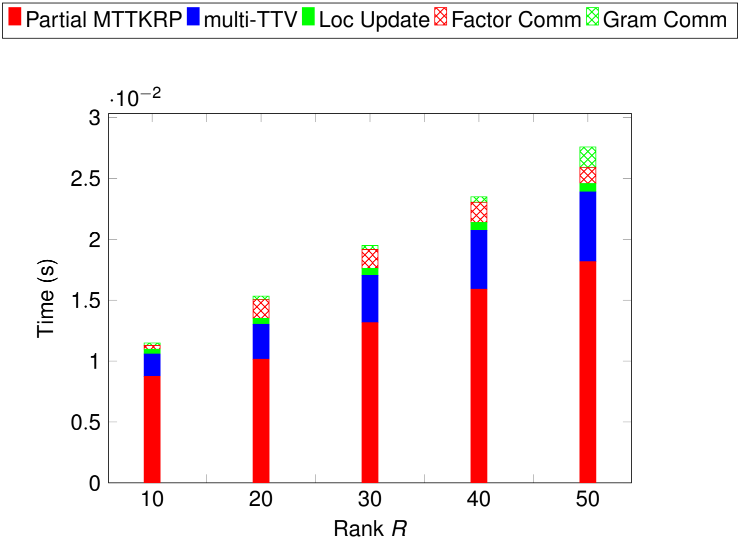

Figure: $1344 \times 1024 \times 33 \times 9$ tensor on $8 \times 8 \times 1 \times 1$ proc grid

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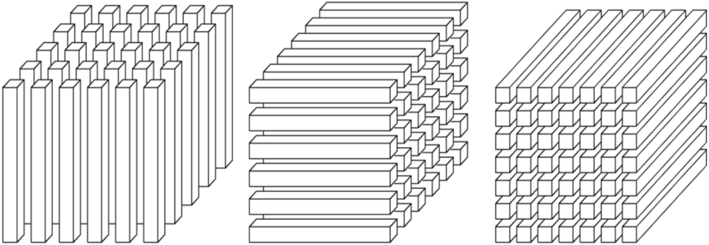
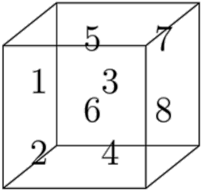
Fibers



Mode-1 Fibers Mode-2 Fibers Mode-3 Fibers

A tensor can be decomposed into the fibers of each mode
(fibers are vectors – fix all indices but one)

$\mathcal{X} =$ 

$$\mathbf{X}_{(1)} = \begin{bmatrix} 1 & 3 & 5 & 7 \\ 2 & 4 & 6 & 8 \end{bmatrix}$$

$$\mathbf{X}_{(2)} = \begin{bmatrix} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \end{bmatrix}$$

$$\mathbf{X}_{(3)} = \begin{bmatrix} 1 & 2 & 3 & 4 \\ 5 & 6 & 7 & 8 \end{bmatrix}$$

A tensor can be reshaped into a matrix,
called a matricized tensor or unfolding, for a given mode,
where each column is a fiber

Sequential Communication Lower Bound

Theorem

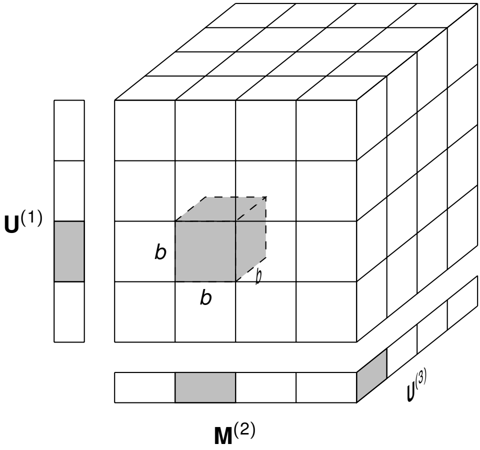
For sufficiently large I, any sequential MTTKRP algorithm performs at least

$$\Omega\left(\frac{NIR}{M^{1-1/N}}\right)$$

loads and stores to/from slow memory.

- N is the number of modes
- I is the number of tensor entries
- R is the rank of the CP model
- M is the size of the fast memory

Communication-Optimal Sequential Algorithm (3D)



1. Loop over $b \times \cdots \times b$ blocks of the tensor

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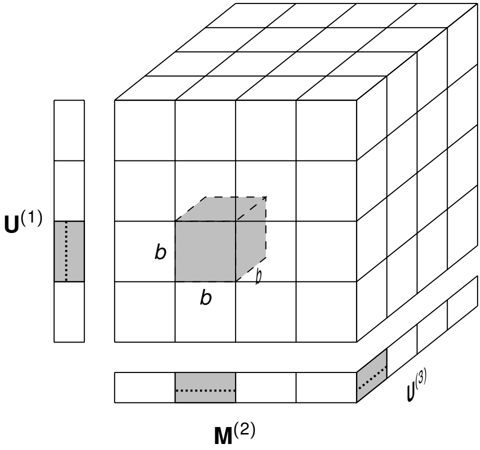

1. Loop over $b \times \cdots \times b$ blocks of the tensor
2. With block in memory, loop over subcolumns of input factor matrices, updating corresponding subcolumn of output matrix

- choose $b \approx M^{1/N}$

Theoretical Comparisons

	Lower Bound	New Algorithm	Standard (MM)
Flops	-	NIR	$2IR$
Words	$\Omega\left(\frac{NIR}{M^{1-1/N}}\right)$	$O\left(I + \frac{NIR}{M^{1-1/N}}\right)$	$O\left(I + \frac{IR}{M^{1/2}}\right)$
Temp Mem	-	-	$\frac{IR}{I_n}$

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Temp Mem	-	-	$\frac{IR}{I_n}$

- New algorithm performs $N/2$ more flops than standard
- For relatively small R, I term dominates communication
  - we expect this to be the typical case in practice
- For relatively large R, new algorithm communicates less
  - better exponent on M

MTTKRP Loop Nest

for $i_1 = 1$ to I_1 **do**

$\ddots$

for $i_N = 1$ to I_N **do**

for $r = 1$ to R **do**

$$\mathbf{M}^{(n)}(i_n, r) \mathrel{+}= \mathcal{X}(i_1, \ldots, i_N) * \mathbf{U}^{(1)}(i_1, r) * \cdots * \mathbf{U}^{(N)}(i_N, r)$$

$$\Delta = \begin{array}{c|cccccc}
 & i_1 & \cdots & i_n & \cdots & i_N & r \\
\hline
\mathbf{U}^{(1)} & 1 & & & & & 1 \\
\vdots & & \ddots & & & & \vdots \\
\mathbf{M}^{(n)} & & & 1 & & & 1 \\
\vdots & & & & \ddots & & \vdots \\
\mathbf{U}^{(N)} & & & & & 1 & 1 \\
\mathcal{X} & 1 & \cdots & 1 & \cdots & 1 &
\end{array}$$