Communication Lower Bounds for Matricized-Tensor Times Khatri-Rao Product

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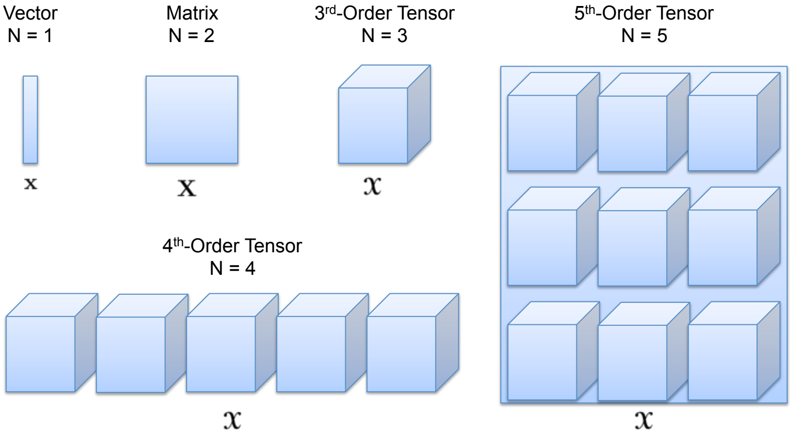
Summary

- We apply the communication lower bound approach for general loop nests to a particular tensor computation: matricized-tensor times Khatri-Rao product (MTTKRP)
  - establishing lower bounds for sequential and parallel cases
- We present optimal algorithms for dense tensors
  - separate algorithms for sequential and parallel cases
  - they attain the lower bounds to within constant factors
- We compare with MTTKRP via matrix multiplication
  - new algorithms may perform more computation
  - they can perform less communication

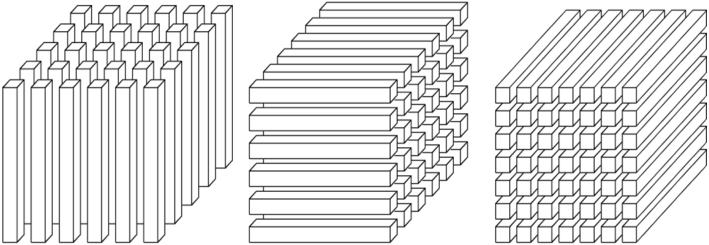
Tensors



An N^{th}-order tensor has N modes

Notation convention: vector **v**, matrix **M**, tensor $\mathcal{X}$

Fibers

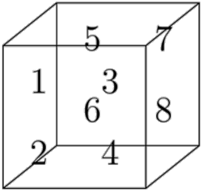


Mode-1 Fibers Mode-2 Fibers Mode-3 Fibers

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

Matricized Tensors

$\mathcal{X} =$



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

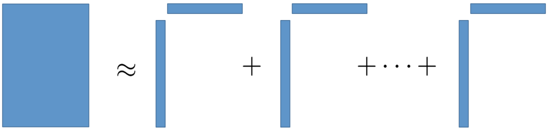
$$\mathbf{X}_{(2)} = \begin{bmatrix} 1 & 2 & 5 & 6 \\ 3 & 4 & 7 & 8 \end{bmatrix}$$

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

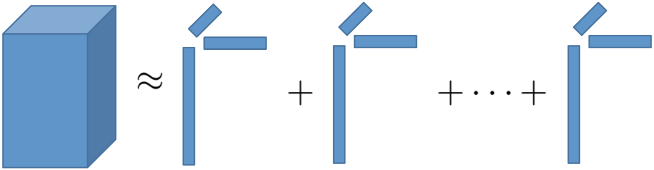
A tensor can be reshaped into a matrix,
called a matricized tensor or unfolding, for a given mode,
where each column is a fiber

CP Decomposition: sum of outer products

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

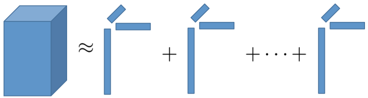


Tensor: $\mathcal{X} \approx \sum_{r=1}^{R} \mathbf{u}_r \circ \mathbf{v}_r \circ \mathbf{w}_r$



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

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

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 element-wise product

All optimization schemes that compute the gradient must also compute MTTKRP in all modes

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

We'll consider alternative approaches that don't form 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**

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

Lower Bounds for MTTKRP

MTTKRP is a set of nested loops that accesses arrays...
... we just learned how to prove communication lower bounds!

From Nick's talk...

- tabulate how the arrays are accessed
- use Hölder-Brascamp-Lieb-type inequality in LB proof
- solve linear program to get tightest lower bound
- details in [CDK$^+$13]

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**

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

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

MTTKRP Lower Bound Proofs

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- Key assumption: algorithm is not allowed to pre-compute and re-use temporary values
  - e.g., forming explicit Khatri-Rao product
- Also used inspiration from memory-independent LBs for matrix multiplication [BDH$^+$12, DEF$^+$13] for parallel case

Sequential Communication Lower Bound

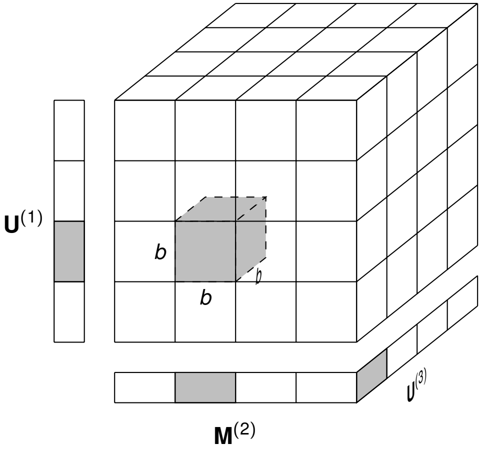
Theorem

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

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

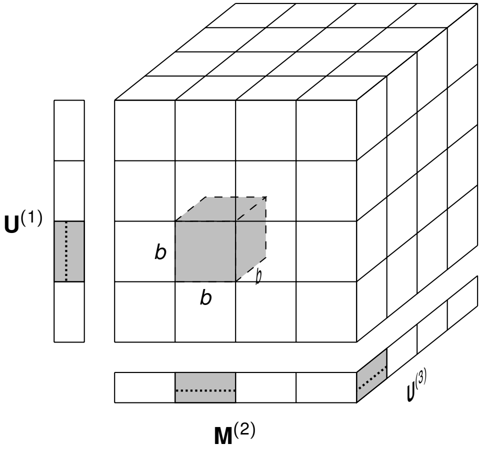
loads and stores to/from slow memory.

- 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



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

Communication-Optimal Sequential Algorithm (3D)



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

Parallel Communication Lower Bound

Theorem

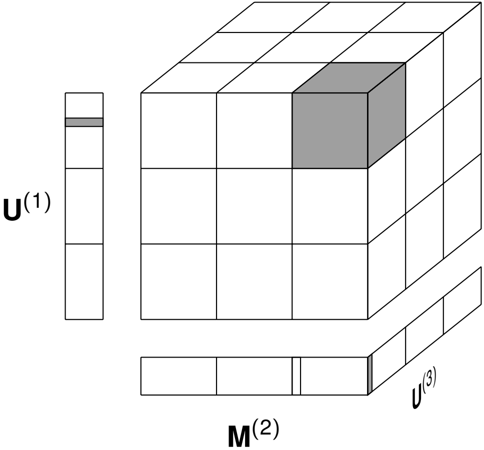
Any parallel MTTKRP algorithm involving a tensor with $I_k = I^{1/N}$ for all k and that evenly distributes one copy of the input and output performs at least

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

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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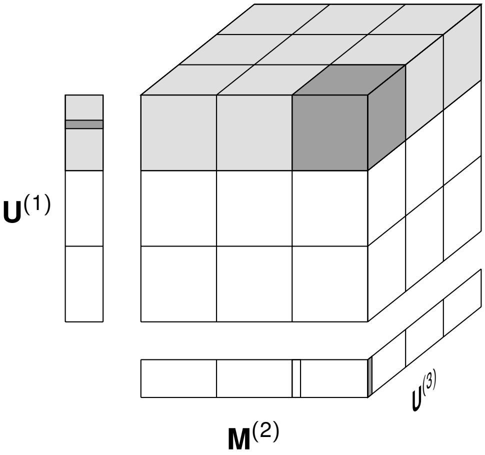

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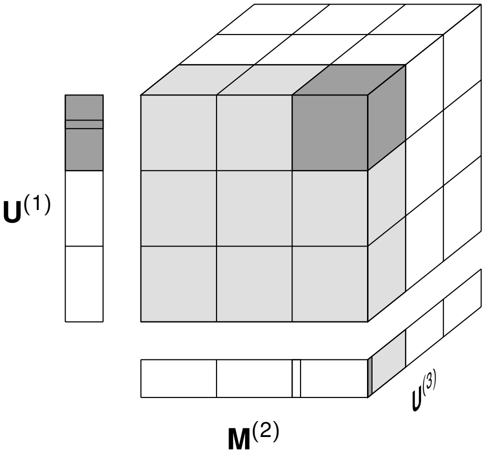

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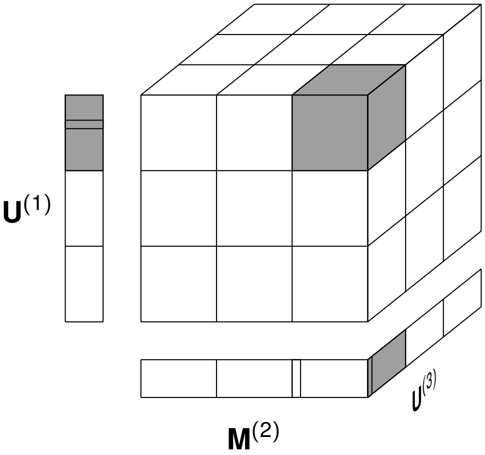

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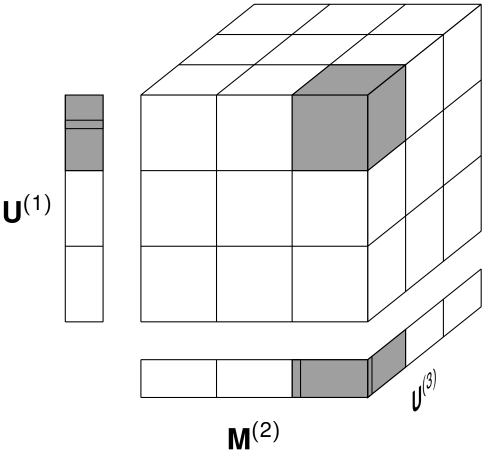
4. Computes its contribution to rows of $\mathbf{M}^{(2)}$ (local MTTKRP)

Communication-Optimal Parallel Algorithm (3D)



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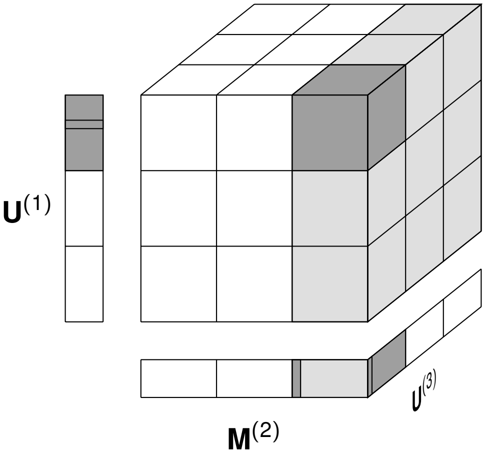

Each processor

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3. All-Gathers all the rows needed from $\mathbf{U}^{(3)}$
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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 algorithm attains lower bound
- Comparison with matrix multiplication from [DEF$^+$13]
  - ignores parallel cost of forming Khatri-Rao product

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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 algorithm attains lower bound
- Comparison with matrix multiplication from [DEF$^+$13]
  - ignores parallel cost of forming Khatri-Rao product
- For larger P (or R), then we need different algorithm
  - also parallelize over columns of output matrix
  - involves communicating the tensor

Summary

- We apply the communication lower bound approach for general loop nests to a particular tensor computation: matricized-tensor times Khatri-Rao product (MTTKRP)
  - establishing lower bounds for sequential and parallel cases
- We present optimal algorithms for dense tensors
  - separate algorithms for sequential and parallel cases
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  - new algorithms may perform more computation
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What about lower bounds for...

- all N MTTKRPs?
  - in sequence, as in CP-ALS
  - all at once, as in gradient-based methods
- partial MTTKRPs and multi-TTVs?
  - MTTKRP methods that violate key assumption
  - [PTC13, KU16, LCP$^+$17]
- other tensor computations like tensor-times-matrix?
  - useful for Tucker decomposition

We believe the same lower bound framework will work, still working out the details

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