Multiple Tensor Times Matrix computation

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CR12: October 2024 https://surakuma.github.io/courses/daamtc.html

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Tucker decomposition of $\mathfrak{X} \in \mathbb{R}^{n_1 imes n_2 imes \cdots imes n_d}$

It represents a tensor with d matrices (usually orthonormal) and a small core tensor.



Tucker decomposition of a 3-dimensional tensor.

$$\mathfrak{X} = \mathfrak{Y} \times_1 \mathsf{A}^{(1)} \cdots \times_d \mathsf{A}^{(d)}$$
$$\mathfrak{X}(i_1, \cdots, i_d) = \sum_{\alpha_1=1}^{i_1} \cdots \sum_{\alpha_d=1}^{i_d} \mathfrak{Y}(\alpha_1, \cdots, \alpha_d) \mathsf{A}^{(1)}(i_1, \alpha_1) \cdots \mathsf{A}^{(d)}(i_d, \alpha_d)$$

It can be concisely expressed as $\mathfrak{X} = [\![\mathfrak{Y} ; \mathsf{A}^{(1)}, \cdots, \mathsf{A}^{(d)}]\!].$

Here r_j for $1 \le j \le d$ denote a set of ranks. Matrices $A^{(j)} \in \mathbb{R}^{n_j \times r_j}$ for $1 \le j \le d$ are usually orthonormal and known as factor matrices. The tensor $\mathcal{Y} \in \mathbb{R}^{r_1 \times r_2 \times \cdots \times r_d}$ is called the core tensor.

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Algorithm 1 HOSVD method to compute a Tucker decomposition

Require: input tensor
$$\mathfrak{X} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$$
, desired rank (r_1, \cdots, r_d)
Ensure: $\mathfrak{X} = \mathfrak{Y} \times_1 A^{(1)} \times_2 A^{(2)} \cdots \times_d A^{(d)}$

- 1: for k = 1 to d do
- 2: $A^{(k)} \leftarrow r_k$ leading left singular vectors of $X_{(k)}$
- 3: end for
- 4: $\mathcal{Y} = \mathcal{X} \times_1 \mathsf{A}^{(1)^\mathsf{T}} \times_2 \mathsf{A}^{(2)^\mathsf{T}} \cdots \times_d \mathsf{A}^{(d)^\mathsf{T}}$

- When $r_i < rank(X_{(i)})$ for one or more *i*, the decomposition is called the truncated-HOSVD (T-HOSVD)
- The collective operation $\mathfrak{X} \times_1 A^{(1)^T} \times_2 A^{(2)^T} \cdots \times_d A^{(d)^T}$ is known as Multiple Tensor-Times-Matrix (Multi-TTM) computation

Sequentially T-HOSVD (ST-HOSVD) for Tucker decomposition

- This method is more work efficient than T-HOSVD
- In each step, it reduces the size of one dimension of the tensor

Algorithm 2 ST-HOSVD method to compute a Tucker decomposition

Require: input tensor $\mathfrak{X} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$, desired rank (r_1, \cdots, r_d) **Ensure:** $[\![\mathfrak{Y}; A^{(1)}, \cdots, A^{(d)}]\!]$: a (r_1, \cdots, r_d) -rank Tucker decomposition of \mathfrak{X} 1: $\mathcal{W} \leftarrow \mathfrak{X}$ 2: for k = 1 to d do 3: $A^{(k)} \leftarrow r_k$ leading singular vectors of $W_{(k)}$ 4: $\mathcal{W} \leftarrow \mathcal{W} \times_k A^{(k)^{\mathsf{T}}}$ 5: end for 6: $\mathcal{Y} = \mathcal{W}$

We can note that ST-HOSVD also performs Multi-TTM computation by doing a sequence of TTM operations, i.e, $\mathcal{Y} = ((\mathcal{X} \times_1 A^{(1)^T}) \times_2 A^{(2)^T}) \cdots \times_d A^{(d)^T}$.

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• Multi-TTM becomes the overwhelming bottleneck computation when

- Matrix SVD costs are reduced using randomization via sketching or
- A^(k) are computed with eigen value decompositions of $X_{(k)}X_{(k)}^{T}$ (or $W_{(k)}W_{(k)}^{T}$)

Multi-TTM computation

Let $\mathcal{Y} \in \mathbb{R}^{r_1 \times \cdots \times r_d}$ be the output tensor, $\mathfrak{X} \in \mathbb{R}^{n_1 \times \cdots \times n_d}$ be the input tensor, and $A^{(k)} \in \mathbb{R}^{n_k \times r_k}$ be the matrix of the *k*th mode. Then the Multi-TTM computation can be represented as $\mathcal{Y} = \mathfrak{X} \times_1 A^{(1)}{}^{\mathsf{T}} \cdots \times_d A^{(d)}{}^{\mathsf{T}}$

or
$$\mathfrak{X} = \mathfrak{Y} \times_1 \mathsf{A}^{(1)} \cdots \times_d \mathsf{A}^{(d)}.$$

We will focus only on the first representation in this course. Our results and analysis extend straightforwardly to the latter case. *Two approaches to perform this computation*:

• TTM-in-sequence approach – performed by a sequence of TTM operations

$$\boldsymbol{\mathcal{Y}} = ((\boldsymbol{\mathfrak{X}} \times_1 \boldsymbol{\mathsf{A}^{(1)}}^\mathsf{T}) \times_2 \boldsymbol{\mathsf{A}^{(2)}}^\mathsf{T}) \cdots \times_d \boldsymbol{\mathsf{A}^{(d)}}^\mathsf{T}$$

All-at-once approach

$$\mathfrak{Y}(r'_1,\ldots,r'_d)=\sum_{\{n'_k\in[n_k]\}_{k\in[d]}}\mathfrak{X}(n'_1,\ldots,n'_d)\prod_{j\in[d]}\mathsf{A}^{(j)}(n'_j,r'_j)$$

[d] denotes $\{1, 2, \dots, d\}$. We represent $n_1 n_2 \cdots n_d$ and $r_1 r_2 \cdots r_d$ by n and r, respectively. We mainly focus on all-at-once approach, $n \in \mathbb{R}$ and $r \in \mathbb{R}$.

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All-at-once Multi-TTM pseudo code

for
$$n'_1 = 1:n_1, \ldots$$
, for $n'_d = 1:n_d$,
for $r'_1 = 1:r_1, \ldots$, for $r'_d = 1:r_d$,
 $\mathcal{Y}(r'_1, \ldots, r'_d) + = \mathcal{X}(n'_1, \ldots, n'_d) \cdot \mathsf{A}^{(1)}(n'_1, r'_1) \cdots \cdot \mathsf{A}^{(N)}(n'_d, r'_d)$



Question: Let $\mathcal{Y} \in \mathbb{R}^{r \times r \times r}$, $\mathcal{X} \in \mathbb{R}^{n \times n \times n}$ and $A \in \mathbb{R}^{n \times r}$. What are the different approaches to perform the following Multi-TTM computation?

$$\mathcal{Y} = \mathfrak{X} imes_1 A^\mathsf{T} imes_2 A^\mathsf{T} imes_3 A^\mathsf{T}$$

Compute the exact number of arithmetic operations for each approach.

1 Parallel Multi-TTM computation

Settings to compute parallel communication lower bound

- Without loss of generality, we assume that $n_1r_1 \leq n_2r_2 \leq \cdots \leq n_dr_d$
- The input tensor is larger than the output tensor, i.e., $n \ge r$
- The algorithm load balances the computation each processor performs $1/P{\rm th}$ number of loop iterations
- One copy of data is in the system
 - There exists a processor whose input data at the start plus output data at the end must be at most $\frac{n+r+\sum_{i=1}^{d} n_i r_i}{p}$ words will analyze amount of data transfers for this processor
- Assume that the innermost computation is atomic all the multiplications are performed on only one processor



Parallel Multi-TTM computation

- 3-dimensional Multi-TTM
- d-dimensional Multi-TTM

Optimization problems (Ballard et. al., 2023)

Lemma

Consider the following optimization problem:

$$\min_{x,y,z} x + y + z \text{ such that}$$

$$\frac{nr}{P} \leq xyz, \quad 0 \leq x \leq n_1r_1, \quad 0 \leq y \leq n_2r_2, \quad 0 \leq z \leq n_3r_3,$$

where $n_1r_1 \le n_2r_2 \le n_3r_3$, and $n_1, n_2, n_3, r_1, r_2, r_3, P \ge 1$. The optimal solution (x^*, y^*, z^*) depends on the relative values of the constraints, yielding three cases:

1 if
$$P < \frac{n_3 r_3}{n_2 r_2}$$
, then $x^* = n_1 r_1$, $y^* = n_2 r_2$, $z^* = \frac{n_3 r_3}{P}$;
2 if $\frac{n_3 r_3}{n_2 r_2} \le P < \frac{n_2 n_3 r_2 r_3}{n_1^2 r_1^2}$, then $x^* = n_1 r_1$, $y^* = z^* = \left(\frac{n_2 n_3 r_2 r_3}{P}\right)^{\frac{1}{2}}$;
3 if $\frac{n_2 n_3 r_2 r_3}{n_1^2 r_1^2} \le P$, then $x^* = y^* = z^* = \left(\frac{nr}{P}\right)^{\frac{1}{3}}$;

which can be visualized as follows.

Lemma

Consider the following optimization problem:

 $\min_{u,v} u + v \text{ such that}$

$$\frac{nr}{P} \leq uv, \quad 0 \leq u \leq r, \quad 0 \leq v \leq n,$$

where $n \ge r$, and $n, r, P \ge 1$. The optimal solution (u^*, v^*) depends on the relative values of the constraints, yielding two cases:

which can be visualized as follows.

$$\begin{array}{cccc}
 & u^* = r & & & & & \\ & u^* = r & & & & \\ & v^* = \frac{n}{P} & & & & & u^* = \left(\frac{nr}{P}\right)^{1/2} \end{array} \xrightarrow{P}$$

Both lemma can be proved using the KKT conditions.

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Theorem

Any computationally load balanced atomic Multi-TTM algorithm that starts and ends with one copy of the data distributed across processors involving 3-dimensional tensors with dimensions n_1, n_2, n_3 and r_1, r_2, r_3 performs at least $A + B - \left(\frac{n}{P} + \frac{r}{P} + \sum_{j=1}^{3} \frac{n_j r_j}{P}\right)$ sends or receives where

$$A = \begin{cases} n_1 r_1 + n_2 r_2 + \frac{n_3 r_3}{P} & \text{if } P < \frac{n_3 r_3}{n_2 r_2} \\ n_1 r_1 + 2 \left(\frac{n_2 n_3 r_2 r_3}{P}\right)^{\frac{1}{2}} & \text{if } \frac{n_3 r_3}{n_2 r_2} \le P < \frac{n_2 n_3 r_2 r_3}{n_1^2 r_1^2} \\ 3 \left(\frac{n_r}{P}\right)^{\frac{1}{3}} & \text{if } \frac{n_2 n_3 r_2 r_3}{n_1^2 r_1^2} \le P \end{cases}$$
$$B = \begin{cases} r + \frac{n}{P} & \text{if } P < \frac{n}{r} \\ 2 \left(\frac{n_r}{P}\right)^{\frac{1}{2}} & \text{if } \frac{n}{r} \le P. \end{cases}$$

Communication lower bound proof

Let *F* be the set of loop indices performed by a processor and |F| = nr/P. Define $\phi_{\mathfrak{X}}(F)$, $\phi_{\mathfrak{Y}}(F)$ and $\phi_j(F)$ to be the projections of *F* onto the indices of the arrays $\mathfrak{X}, \mathfrak{Y}$, and $A^{(j)}$ for $1 \leq j \leq 3$. Δ matrix can be represented as,

$$\Delta = \begin{pmatrix} \mathsf{I}_{3\times3} & \mathsf{1}_3 & \mathsf{0}_3 \\ \mathsf{I}_{3\times3} & \mathsf{0}_3 & \mathsf{1}_3 \end{pmatrix}.$$

Let $C = \{s \in [0,1]^5 : \Delta \cdot s \ge 1\}$. Here Δ is not full rank, we consider all vectors $v = [a \ a \ a \ 1-a]^T \in C$ where $0 \le a \le 1$ such that $\Delta \cdot v = 1$. From HBL inequality, we obtain

$$\frac{nr}{P} \leq \Big(\prod_{j\in[3]} |\phi_j(F)|\Big)^{\mathfrak{s}} \big(|\phi_{\mathfrak{X}}(F)||\phi_{\mathfrak{Y}}(F)|\big)^{1-\mathfrak{s}}.$$

This is equivalent to $\frac{nr}{P} \leq \prod_{j \in [3]} |\phi_j(F)|$ and $\frac{nr}{P} \leq |\phi_X(F)| |\phi_y(F)|$. We also have $|\phi_X(F)| \leq n$, $|\phi_y(F)| \leq r$, and $|\phi_j(F)| \leq n_j r_j$ for $1 \leq j \leq 3$. We want to minimize $|\phi_X(F)| + |\phi_y(F)| + \sum_{j \in [3]} |\phi_j(F)|$. Employing the previous two lemmas and subtracting the owned data of the processor yields the mentioned bound.

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Corollary

Any computationally load balanced atomic Multi-TTM algorithm that starts and ends with one copy of the data distributed across processors involving 3-dimensional cubical tensors with dimensions $n^{\frac{1}{3}} \times n^{\frac{1}{3}} \times n^{\frac{1}{3}}$ and $r^{\frac{1}{3}} \times r^{\frac{1}{3}} \times r^{\frac{1}{3}}$ (with $n \ge r$) performs at least

$$3\left(\frac{nr}{P}\right)^{\frac{1}{3}}+r-\frac{3(nr)^{\frac{1}{3}}+r}{P}$$

sends or receives when $P < \frac{n}{r}$ and at least

$$3\left(\frac{nr}{P}\right)^{\frac{1}{3}} + 2\left(\frac{nr}{P}\right)^{\frac{1}{2}} - \frac{n+3(nr)^{\frac{1}{3}}+r}{P}$$

sends or receives when $P \geq \frac{n}{r}$.

We will manily focus on $P < \frac{n}{r}$ case throughout the slides.

P processors are organized in a 6-dimensional $p_1 \times p_2 \times p_3 \times q_1 \times q_2 \times q_3$ logical processor grid.



Subtensor \mathfrak{X}_{231} is distributed evenly among processors (2, 3, 1, *, *, *). Similarly, submatrix $A_{31}^{(2)}$ is distributed evenly among processors (*, 3, *, *, 1, *).

Algorithm 3 Parallel Atomic 3-dimensional Multi-TTM

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Require: \mathfrak{X}, A^{(1)}, A^{(2)}, A^{(3)}, p_1 \times p_2 \times p_3 \times q_1 \times q_2 \times q_3 logical processor grid Ensure: \mathfrak{Y} such that \mathfrak{Y} = \mathfrak{X} \times_1 A^{(1)^{\mathsf{T}}} \times_2 A^{(2)^{\mathsf{T}}} \times_3 A^{(3)^{\mathsf{T}}}
  1: (p'_1, p'_2, p'_3, q'_1, q'_2, q'_3) is my processor id
  2: //All-gather input tensor \mathfrak{X}
  3: \mathfrak{X}_{p'_1p'_2p'_3} = \mathsf{All-Gather}(\mathfrak{X}, (p'_1, p'_2, p'_3, *, *, *))
  4: //All-gather input matrices
  5: A_{p'_{1}q'_{1}}^{(1)} = All-Gather(A^{(1)}, (p'_{1}, *, *, q'_{1}, *, *))
  6: A_{p'_2q'_2}^{(2)} = \text{All-Gather}(A^{(2)}, (*, p'_2, *, *, q'_2, *))
  7: A^{(3)}_{p'_3 q'_3} = All-Gather(A^{(3)}, (*, *, p'_3, *, *, q'_3))
  8: //Local computations in a temporary tensor \mathfrak{T}
  9: \mathfrak{T} = \text{Local-Multi-TTM}(\mathfrak{X}_{\rho'_1\rho'_2\rho'_3}, \mathsf{A}^{(1)}_{\rho'_2\rho'_3}, \mathsf{A}^{(2)}_{\rho'_2\sigma'_2}, \mathsf{A}^{(3)}_{\rho'_2\sigma'_2})
10: //Reduce-scatter the output tensor in \mathcal{Y}_{q_1'q_2'q_3'}
11: Reduce-Scatter(\mathcal{Y}_{q'_1q'_2q'_2}, \mathcal{T}, (*, *, *, q'_1, q'_2, q'_3))
```

Steps of the algorithm



Steps of the algorithm for processor (2, 1, 1, 1, 3, 1), where $p_1 = p_2 = p_3 = q_1 = q_2 = q_3 = 3$. Highlighted areas correspond to the data blocks on which the processor is operating. The dark red highlighting represents the input/output data initially/finally owned by the processor, and the light red highlighting corresponds to received/sent data from/to other processors in All-Gather/Reduce-Scatter collectives to compute \mathcal{Y}_{131} .

Cost analysis

The bandwidth cost of the algorithm is

$$\frac{n}{p} + \frac{n_1 r_1}{p_1 q_1} + \frac{n_2 r_2}{p_2 q_2} + \frac{n_3 r_3}{p_3 q_3} + \frac{r}{q} - \left(\frac{n + n_1 r_1 + n_2 r_2 + n_3 r_3 + r}{P}\right).$$

Here $p = p_1 p_2 p_3$ and $q = q_1 q_2 q_3$. The algorithm is communication optimal when we select p_i and q_i based on lower bounds.

Arithmetic operations

The dimensions of $\mathfrak{X}_{p'_1p'_2p'_3}$ and \mathfrak{T} are $\frac{n_1}{p_1} \times \frac{n_2}{p_2} \times \frac{n_3}{p_3}$ and $\frac{r_1}{q_1} \times \frac{r_2}{q_2} \times \frac{r_3}{q_3}$, respectively. The dimension of $\mathsf{A}_{p'_kq'_k}^{(k)}$ is $\frac{n_i}{p_i} \times \frac{r_i}{q_i}$ for i = 1, 2, 3.

- Local Multi-TTM can be performed as a sequence of TTM operations
- Assuming TTM operations are performed in their order, first with $A^{(1)},$ then with $A^{(2)},$ and in the end with $A^{(3)},$

Total arithmetic operations
$$= 2\left(\frac{n_1n_2n_3r_1}{p_1p_2p_3q_1} + \frac{n_2n_3r_1r_2}{p_2p_3q_1q_2} + \frac{n_3r_1r_2r_3}{p_3q_1q_2q_3}\right).$$

Multi-TTM cost in TuckerMPI library

- State-of-the-art library for parallel Tucker decomposition
- Implements ST-HOSVD algorithm employs TTM-in-sequence approach to perform Multi-TTM
- Assume TTMs are performed in increasing mode order

It uses a $\tilde{p_1}\times\tilde{p_2}\times\tilde{p_3}$ logical processor grid. The bandwidth cost is

$$\frac{r_1n_2n_3}{\tilde{p}_2\tilde{p}_3} + \frac{n_1r_1}{\tilde{p}_1} + \frac{r_1r_2n_3}{\tilde{p}_1\tilde{p}_3} + \frac{n_2r_2}{\tilde{p}_2} + \frac{r_1r_2r_3}{\tilde{p}_1\tilde{p}_2} + \frac{n_3r_3}{\tilde{p}_3} - \frac{r_1n_2n_3 + r_1r_2n_3 + r_1r_2r_3 + n_1r_1 + n_2r_2 + n_3r_3}{P}$$

The parallel computational cost is

$$2\left(\frac{r_1n_1n_2n_3 + r_1r_2n_2n_3 + r_1r_2r_3n_3}{P}\right)$$



Communication cost comparison of all-at-once approach (the presented algorithm) and TTM-in-sequence approach (of TuckerMPI). *Comp-Overhead* shows the percentage of computational overhead of the all-at-once approach with respect to the TTM-in-sequence approach. Cost of an approach represents the minimum cost among all possible processor configurations.

Comparison of All-at-once and TTM-in-sequence



- Not any clear winner for all settings
- All-at-once approach performs significantly less communication for small P
- Computational overhead of all-at-once approach is negligible for small P
- TTM-in-sequence approach is better for large P



Parallel Multi-TTM computation

- 3-dimensional Multi-TTM
- d-dimensional Multi-TTM

Theorem

Any computationally load balanced atomic Multi-TTM algorithm that starts and ends with one copy of the data distributed across processors and involves d-dimensional tensors with dimensions n_1, n_2, \ldots, n_d and r_1, r_2, \ldots, r_d performs at least $A + B - \left(\frac{n}{P} + \frac{r}{P} + \sum_{j=1}^{d} \frac{n_j r_j}{P}\right)$ sends or receives where

$$A = \begin{cases} \sum_{j=1}^{d-1} n_j r_j + \frac{N_1 R_1}{P} & \text{if } P < \frac{N_1 R_1}{n_{d-1} r_{d-1}}, \\ \sum_{j=1}^{(d-i)} n_j r_j + i \left(\frac{N_i R_i}{P}\right)^{\frac{1}{7}} & \text{if } \frac{N_{i-1} R_{i-1}}{(n_{d+1-i} r_{d+1-i})^{r-1}} \le P < \frac{N_i R_i}{(n_{d-i} r_{d-i})^{j}}, \\ for some \ 2 \le i \le d-1, \\ d \left(\frac{N_d R_d}{P}\right)^{\frac{1}{d}} & \text{if } \frac{N_{d-1} R_{d-1}}{(n_1 r_1)^{d-1}} \le P. \end{cases}$$
$$B = \begin{cases} r + \frac{n}{P} & \text{if } P < \frac{n}{r}, \\ 2 \left(\frac{nr}{P}\right)^{\frac{1}{2}} & \text{if } \frac{n}{r} \le P. \end{cases}$$

Parallel Multi-TTM algorithm

Algorithm 4 Parallel Atomic d-dimensional Multi-TTM

Require:
$$\mathfrak{X}$$
, $A^{(1)}$, ..., $A^{(d)}$, $p_1 \times \cdots \times p_d \times q_1 \times \cdots \times q_d$ logical processor grid
Ensure: \mathfrak{Y} such that $\mathfrak{Y} = \mathfrak{X} \times_1 A^{(1)^{\mathsf{T}}} \cdots \times_d A^{(d)^{\mathsf{T}}}$
1: $(p'_1, \cdots, p'_d, q'_1, \cdots, q'_d)$ is my processor id
2: $//\text{All-gather input tensor } \mathfrak{X}$
3: $\mathfrak{X}_{p'_1 \cdots p'_d} = \text{All-Gather}(\mathfrak{X}, (p'_1, \cdots, p'_d, *, \cdots, *))$
4: $//\text{All-gather all input matrices}$
5: for $i = 1, \cdots, d$ do
6: $A^{(i)}_{p'_i q'_i} = \text{All-Gather}(A^{(i)}, (*, \cdots, *, p'_i, *\cdots, *, q'_i, *))$
7: end for
8: $//\text{Perform local computations in a temporary tensor } \mathfrak{T}$
9: $\mathfrak{T} = \text{Local-Multi-TTM}(\mathfrak{X}_{p'_1 \cdots p'_d}, A^{(1)}_{p'_1 q'_1}, \cdots, A^{(d)}_{p'_d q'_d})$
10: $//\text{Reduce-scatter the output tensor in $\mathfrak{Y}_{q'_1 \cdots q'_d}$
11: Reduce-Scatter($\mathfrak{Y}_{q'_1 \cdots q'_d}, \mathfrak{T}, (*, \cdots, *, q'_1, \cdots, q'_d)$)$

The algorithm is communication optimal when p_i and q_i are selected based on the lower bound.

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- Cost analysis of several ways to perform Multi-TTM
 - Unifying all-at-once and sequence approaches
 - Study of communication-computation trade-off

- Optimal costs for algorithms to compute Tucker decompositions
- Design and implementation of parallel optimal algorithms