Fast Layout-Oblivious Tensor-Matrix Multiplication with BLAS

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Abstract. The tensor-matrix multiplication is a basic tensor operation that is required by various tensor methods such as the ALS or the HOSVD. This paper presents flexible high-performance algorithms that compute the tensor-matrix product according to the Loops-over-gemms (LOG) approach. Our algorithms can process dense tensors with any linear tensor layout, arbitrary tensor order and dimensions all of which can be runtime variable. We discuss different tensor slicing methods with parallelization strategies and propose six versions which call `gemv`, `gemm` and/or `gemm_batch` with subtensors or tensor slices. Their performance is quantified for a set of tensors with various shapes and tensor order. Our best performing version attains a median performance of 1.37 double precision Tflops on an Intel Xeon Gold 6248R processor using Intel's MKL. We show that the performance is only slightly affected by the tensor layout and the median performance is between [?] and [?] Tflops for a range of linear tensor formats. Our fastest implementation is on average at least by 14.05% and up to 3.79 x faster than other state-of-the-art implementations, including Libtorch and Eigen.

1 Introduction

Tensor computations are found in many scientific fields such as computational neuroscience, pattern recognition, signal processing and data mining [5,12]. Tensors representing large amount of multidimensional data are decomposed and analyzed with the help of basic tensor operations [6,7]. The decomposition and analysis led to the development and analysis of high-performance kernels for tensor contractions. In this work, we present and analyze a high-performance algorithm for the tensor-matrix multiplication that is used in many numerical algorithms such as the alternating least squares method [6,7]. It is a compute-bound tensor operation and has the same arithmetic intensity as a matrix-matrix multiplication which can almost reach the practical peak performance of a computing machine.

There has been three main approaches for implementing tensor contractions. The Transpose-Transpose-`gemm`-Transpose (TGGT) approach reorganizes (flattens) tensors in order to perform a tensor contraction with an optimized matrix-matrix multiplication (`gemm`) implementation [1,14]. Implementations of the GETT method are based on high-performance `gemm`-like algorithms [10,15].

A different method is the LOG approach in which BLAS are utilized with multiple tensor slices or subtensors if possible [8, 11, 13]. Implementations of the LOG and TTGT approaches are in general easier to maintain and faster to port than GETT implementations which might need to adapt vector instructions or blocking parameters according to a processor's microarchitecture.

To our best knowledge, we are the first to combine the approach described in [2] with the findings on tensor slicing in [8] and to propose fast in-place algorithms that are layout-oblivious. Our algorithms compute the tensor-matrix product in parallel together with highly efficient `gemm` or `gemm_batch` implementations. They support dense tensors with any order, dimensions and any linear tensor layout including the first- and the last-order storage formats for any contraction mode all of which can be runtime variable. Input and output tensors do not need to be transposed or flattened into two-dimensional matrices. The parallel versions of the recursive base algorithm execute fused loops in parallel and are able to fully utilize a processors compute units. Despite, the generality of our approach, every proposed algorithm can be implemented with less than 100 lines of `C++` code where the complexity is hidden by the BLAS implementation and the corresponding selection of subtensors or tensor slices. We have provided an open and free reference `C++` implementation of all algorithms and a python interface for convenience. While we have used Intel's MKL for our benchmarks, the user is free to choose any other library that provides the BLAS interface.

The following analysis quantifies the impact of the tensor layout, the tensor slicing method and parallel execution of slice-matrix multiplications with varying contraction modes. The runtime measurements of our implementations are compared with those presented in [10, 15] including Libtorch and Eigen. In summary, the main findings of our work are:

- A tensor-matrix multiplication can be implemented by an in-place algorithm with 1 `gemv` and 7 `gemm` calls supporting all combinations of contraction mode, tensor order and dimensions for any linear tensor layout.
- Our algorithm with variable loop fusion and parallel slice-matrix multiplications is on average 17% faster than Intel's `gemm_batch` when the contraction and leading dimensions of the tensors are greater than 256.
- Our algorithms are layout oblivious. The fastest implementations achieve at least a median throughput of [?] for any linear tensor layout.
- Our fastest algorithm computes the tensor-matrix multiplication on average, by at least by 14.05% and up to a factor of 3.79 faster than other state-of-the art library implementations, including LibTorch and Eigen.

The remainder of the paper is organized as follows. Section 2 presents related work. Section 3 introduces some notation on tensors and defines the tensor-matrix multiplication. Algorithm design and methods for slicing and parallel execution are discussed in Section 4. Section 5 describes the test setup. Benchmark results are presented in Section 6. Conclusions are drawn in Section 7.

2 Related Work

The authors in [11] discuss the efficient tensor contractions with highly optimized `BLAS`. Based on the `LOG` approach, they define requirements for the use of `GEMM` for class 3 tensor contractions and provide slicing techniques for tensors. The slicing recipe for the class 2 categorized tensor contractions contains a short description with a rule of thumb for maximizing performance. Runtime measurements cover class 3 tensor contractions.

The work in [8] presents a framework that generates in-place tensor-matrix multiplication according to the `LOG` approach. The authors present two strategies for efficiently computing the tensor contraction applying `GEMM`s with tensors. They report a speedup of up to 4x over the `TTGT`-based `MATLAB` tensor toolbox library discussed in [1]. Although many aspects are similar to our work, the authors emphasize the code generation of tensor-matrix multiplications using high-performance `GEMM`'s.

The authors of [15] present a tensor-contraction generator `TCCG` and the `GETT` approach for dense tensor contractions that is inspired from the design of a high-performance `GEMM`. Their unified code generator selects implementations from generated `GETT`, `LoG` and `TTGT` candidates. Their findings show that among 48 different contractions 15% of `LoG` based implementations are the fastest. However, their tests do not include the tensor-vector multiplication where the contraction exhibits at least one free tensor index.

Using also the `GETT` approach, the author presents in [10] a runtime flexible tensor contraction library. He describes block-scatter-matrix algorithm which uses a special layout for the tensor contraction. The proposed algorithm yields results that feature a similar runtime behavior to those presented in [15].

3 Background

Notation An order-p tensor is a p-dimensional array [9] where tensor elements are contiguously stored in memory. We write a, $\mathbf{a}$, $\mathbf{A}$ and $\underline{\mathbf{A}}$ in order to denote scalars, vectors, matrices and tensors. If not otherwise mentioned, we assume $\underline{\mathbf{A}}$ to have a tensor order that is greater than 2. The p-tuple $\mathbf{n}$ with $\mathbf{n} = (n_1, n_2, \dots, n_p)$ will be referred to as a dimension tuple with $n_r > 1$. We will use round brackets $\underline{\mathbf{A}}(i_1, i_2, \dots, i_p)$ or $\underline{\mathbf{A}}(\mathbf{i})$ to denote a tensor element where $\mathbf{i} = (i_1, i_2, \dots, i_p)$ is a multi-index. A subtensor is denoted by $\underline{\mathbf{A}}'$ and references elements of a tensor $\underline{\mathbf{A}}$. They are specified with p index ranges and form a selection grid. In this work, the index range shall either address all indices of a given mode or a single element that are given by single indices i_r with $1 \leq r \leq p$. Elements n'_r of a subtensor's dimension tuple $\mathbf{n}'$ are therefore n_r if all indices of mode r are selected and 1 otherwise. We will annotate subtensors using only their non-unit modes such as $\underline{\mathbf{A}}'_{u,v,w}$ where $n_u > 1$,$n_v > 1$ and $n_w > 1$ and $1 \leq u \neq v \neq w \leq p$. It is sufficient to only provide non-unit modes as the remaining single indices correspond to the loop induction variables of the following algorithms. A subtensor is called a slice $\underline{\mathbf{A}}'_{u,v}$ if the full range selection of $\underline{\mathbf{A}}$ occurs with only two modes. A fiber $\underline{\mathbf{A}}'_u$ is a tensor slice with only one dimension greater than 1.

Linear Tensor Layouts We use a layout tuple $\boldsymbol{\pi} \in \mathbb{N}^p$ to encode all linear tensor layouts including the first-order or last-order layout. They contain permuted tensor modes whose priority is given by their index. For instance, the first- and last-order storage formats are given by $\boldsymbol{\pi}_F = (1, 2, \ldots, p)$ and $\boldsymbol{\pi}_L = (p, p-1, \ldots, 1)$. An inverse layout tuple $\boldsymbol{\pi}^{-1}$ is defined by $\boldsymbol{\pi}^{-1}(\boldsymbol{\pi}(k)) = k$. Given a layout tuple $\boldsymbol{\pi}$ with p modes, the π_r-th element of a stride tuple is given by $w_{\pi_r} = \prod_{k=1}^{r-1} n_{\pi_k}$ for $1 < r \leq p$ and $w_{\pi_1} = 1$. Tensor elements of the π_1-th mode are contiguously stored in memory. The location of tensor elements is determined by the tensor layout and the layout function. For a given tensor layout and stride tuple, a layout function $\lambda_{\mathbf{w}}$ maps a multi-index to a scalar index with $\lambda_{\mathbf{w}}(\mathbf{i}) = \sum_{r=1}^{p} w_r(i_r - 1)$. With $j = \lambda_{\mathbf{w}}(\mathbf{i})$ being the relative memory position of an element with a multi-index $\mathbf{i}$, reading from and writing to memory is accomplished with j and the first element's address of $\underline{\mathbf{A}}$.

Non-Modifying Flattening and Reshaping The flattening operation $\varphi_{r,q}$ transforms an order-p tensor $\underline{\mathbf{A}}$ to another order-p' view $\underline{\mathbf{B}}$ that has different a shape $\mathbf{m}$ and layout $\boldsymbol{\tau}$ tuple of length p' with $p' = p - q + r$ and $1 \leq r < q \leq p$. It is related to the tensor unfolding operation as defined in [6, p.459] but neither changes the element ordering nor copies tensor elements. Given a layout tuple $\boldsymbol{\pi}$ of $\underline{\mathbf{A}}$, the flattening operation $\varphi_{r,q}$ is defined for contiguous modes $\hat{\boldsymbol{\pi}} = (\pi_r, \pi_{r+1}, \ldots, \pi_q)$ of $\boldsymbol{\pi}$. Let $j = 0$ if $k \leq r$ and $j = q - r$ otherwise for $1 \leq k \leq p'$. Then the resulting layout tuple $\boldsymbol{\tau} = (\tau_1, \ldots, \tau_{p'})$ of $\underline{\mathbf{B}}$ is given by $\tau_r = \min(\boldsymbol{\pi}_{r,q})$ and $\tau_k = \pi_{k+j} + s_k$ if $k \neq r$ where $s_k = |\{\pi_i \mid \pi_{k+j} > \pi_i \wedge \pi_i \neq \min(\hat{\boldsymbol{\pi}}) \wedge r \leq i \leq p\}|$. Elements of the corresponding shape tuple $\mathbf{m}$ are given by $m_{\tau_r} = \prod_{k=r}^{q} n_{\pi_k}$ and $m_{\tau_k} = n_{\pi_{k+j}}$ if $k \neq r$.

The reshaping operation ρ transforms an order-p tensor $\underline{\mathbf{A}}$ to another order-p tensor $\underline{\mathbf{B}}$ with different shape $\mathbf{m}$ and layout $\boldsymbol{\tau}$ tuples of length p. In this work, it permutes the shape and layout tuple simultaneously without changing the element ordering and without copying tensor elements. The operation ρ uses a permutation tuple $\boldsymbol{\rho} = (\rho_1, \ldots, \rho_p)$ to only modify shape and layout tuples. Elements of the resulting shape tuple $\mathbf{m}$ and the layout tuple $\boldsymbol{\tau}$ are given by $m_r = n_{\rho_r}$ and $\tau_r = \pi_{\rho_r}$, respectively.

Tensor-Matrix Multiplication (TTM) Let $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ be order-p tensors with shapes $\mathbf{n}_a = (n_1, \ldots, n_q, \ldots, n_p)$ and $\mathbf{n}_c = (n_1, \ldots, n_{q-1}, m, n_{q+1}, \ldots, n_p)$. Let $\mathbf{B}$ be a matrix of shape $\mathbf{n}_b = (m, n_q)$. A mode-q TTM is denoted by $\underline{\mathbf{C}} = \underline{\mathbf{A}} \times_q \mathbf{B}$ where an element of $\underline{\mathbf{C}}$ is given by

$$\underline{\mathbf{C}}(i_1, \ldots, i_{q-1}, j, i_{q+1}, \ldots, i_p) = \sum_{i_q=1}^{n_q} \underline{\mathbf{A}}(i_1, \ldots, i_q, \ldots, i_p) \cdot \mathbf{B}(j, i_q) \tag{1}$$

with $1 \leq i_r \leq n_r$ and $1 \leq j \leq m$. The mode q is the *contraction mode* of the TTM with $1 \leq q \leq p$. The tensor-matrix multiplication generalizes the computational aspect of the two-dimensional case $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ if $p = 2$ and $q = 1$.

Its arithmetic intensity is equal to that of a matrix-matrix multiplication and is not memory-bound. In the following, we assume that the tensors $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ have the same tensor layout $\boldsymbol{\pi}$. Elements of matrix $\underline{\mathbf{B}}$ can stored in either the column-major or row-major format.

4 Algorithm Design

4.1 Sequential Algorithm

The sequential baseline algorithm for Eq. 1 can be implemented with a single C++ function that supports tensors with arbitrary order, dimensions and any linear tensor layout. It consists of nested recursion with a control flow that is akin to algorithm 1 in [3] consisting of two `if` statements with an `else` branch. The body of the first `if` statement contains a recursive call that skips the iteration over the dimension n_q when $r = \hat{q}$ with $\pi_r = q$ and $\hat{q} = \boldsymbol{\pi}_q^{-1}$ where $\boldsymbol{\pi}^{-1}$ is the inverse layout tuple. The second `if` statement contains multiple recursive calls for the modes $1 \leq r \neq \hat{q} \leq p$ with different multi-indices. The `else` branch is the base case and consists of two loops that compute a fiber-matrix product. The outer loop iterates with j over the dimension m of $\underline{\mathbf{C}}$ and $\mathbf{B}$. The inner loop iterates with i_q over the dimension n_q of $\underline{\mathbf{A}}$ and $\mathbf{B}$ computing an inner product.

4.2 Baseline Algorithm with Contiguous Memory Access

The baseline algorithm accesses elements of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ non-contiguously whenever $\pi_1 \neq q$. Matrix $\mathbf{B}$ is contiguously accessed if i_q or j is incremented with unit-steps depending on the storage format of $\underline{\mathbf{B}}$. The access pattern can be improved by reordering tensor elements according to the storage format. However, copy operations reduce the overall throughput of the operation [13].

A better approach is to access tensor elements according to the tensor layout using the tensor layout tuple $\boldsymbol{\pi}$ as proposed in [3]. The modified algorithm 1 contiguously accesses memory for $\pi_1 \neq q$ and $p > 1$. Each recursion level adjusts only one multi-index element i_{π_r} with a stride w_{π_r} in line 5. With increasing recursion level and decreasing r, indices are incremented with smaller step sizes as $w_{\pi_r} \leq w_{\pi_{r+1}}$. The condition of the second `if` statement in line 4 is changed from $r \geq 1$ to $r > 1$. In this way, the mode-π_1 loop with index i_{π_1} and the minimum stride w_{π_1} are included in the base case which contains three loops performing a slice-matrix multiplication. The loop ordering are adjusted according to the tensor and matrix layout. The inner-most loop increments i_{π_1} and contiguously accesses tensor elements of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$. The second loop increments i_q with which elements of $\mathbf{B}$ are contiguously accessed if $\mathbf{B}$ is stored in the row-major format. The third loop increments j and could be placed as the second loop if $\mathbf{B}$ is stored in the column-major format.

While spatial data locality is improved by adjusting the loop ordering, the temporal data locality of tensors $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ differ. Note that slice $\underline{\mathbf{A}}'_{\pi_1,q}$ is accessed m times, fiber $\underline{\mathbf{C}}_{\pi_1}$ is accessed $\mathbf{n}(q)$ times and element $\underline{\mathbf{B}}(j, i_q)$ is accessed $\mathbf{n}(\pi_1)$

$\texttt{tensor\_times\_matrix}(\underline{\mathbf{A}}, \mathbf{B}, \underline{\mathbf{C}}, \mathbf{n}, \mathbf{i}, m, q, \hat{q}, r)$
  if $r = \hat{q}$ **then**
    $\texttt{tensor\_times\_matrix}(\underline{\mathbf{A}}, \mathbf{B}, \underline{\mathbf{C}}, \mathbf{n}, \mathbf{i}, m, q, \hat{q}, r-1)$
  else if $r > 1$ **then**
    for $i_{\pi_r} \leftarrow 1$ **to** n_{π_r} **do**
      $\texttt{tensor\_times\_matrix}(\underline{\mathbf{A}}, \mathbf{B}, \underline{\mathbf{C}}, \mathbf{n}, \mathbf{i}, m, q, \hat{q}, r-1)$
  else
    for $j \leftarrow 1$ **to** m **do**
      for $i_q \leftarrow 1$ **to** n_q **do**
        for $i_{\pi_1} \leftarrow 1$ **to** n_{π_1} **do**
          $\underline{\mathbf{C}}(i_1, ..., i_{q-1}, j, i_{q+1}, ..., i_p)$ += $\underline{\mathbf{A}}(i_1, ..., i_q, ..., i_p) \cdot \mathbf{B}(j, i_q)$

Algorithm 1: Modified baseline algorithm with contiguous memory access for the tensor-matrix multiplication. The tensor order must be greater than one and for the contraction mode $1 \leq q \leq p$ and $\pi_1 \neq q$ must hold. The algorithm needs to be initially called with $r = p$ where $\mathbf{n}$ is the shape tuple of $\underline{\mathbf{A}}$ and m is the q-th dimension of $\underline{\mathbf{C}}$.

times. While the specified fiber of $\underline{\mathbf{C}}$ can fit into first or second level cache, slice elements of $\underline{\mathbf{A}}$ are unlikely to fit in the local caches if the slice size $n_{\pi_1} \times n_q$ is large leading to higher cache misses and suboptimal performance. Optimized tiling for better temporal data locality has been discussed in [4] which suggests to use existing high-performance BLAS implementations for the base case.

4.3 BLAS-based Algorithms with Tensor Slices

Algorithm 1 is the starting point for the BLAS-based algorithm which computes the tensor-matrix product with a `gemm` routine. Besides the illustrated algorithm, we have identified seven other cases where a single `gemm` call suffices to compute the tensor-matrix product even if the tensor order $p > 2$. In summary, there are eight cases with a single `gemm` call using different arguments which are listed in table 1. The list of `gemm` calls supports all linear tensor layout and has no limitation on tensor order and contraction mode. The arguments of `gemm` are chosen depending on the tensor order p, tensor layout $\boldsymbol{\pi}$ and contraction mode q except for the `CBLAS_ORDER` which is `CblasRowMajor`.

Case 1 ($p = 1$): The tensor-vector product $\underline{\mathbf{A}} \times_1 \mathbf{B}$ can be computed with a `gemv` operation $\mathbf{a}^T \cdot \mathbf{B}$ where $\underline{\mathbf{A}}$ is an order-1 tensor, i.e. a vector $\mathbf{a}$ of length n_1.

Case 2-5 ($p = 2$): If $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are order-2 tensors, i.e. a matrix $\mathbf{A}$ with dimensions n_1 and n_2, then a single `gemm` suffices to compute the tensor-matrix product. If $\mathbf{A}$ and $\mathbf{C}$ have the column-major format with $\boldsymbol{\pi} = (1, 2)$, `gemm` either executes $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}^T$ for $q = 1$ or $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ for $q = 2$. Note that `gemm` interprets $\mathbf{C}$ and $\mathbf{A}$ as matrices using the reshaping operation ρ with $\boldsymbol{\rho} = (2, 1)$ in row-major format even though both are stored column-wise. If $\mathbf{A}$ and $\mathbf{C}$ have the row-major format with $\boldsymbol{\pi} = (2, 1)$, `gemm` either executes $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ for $q = 1$ or

Case	Order p	Layout $\boldsymbol{\pi}$	Mode q	Routine	`T`	`M`	`N`	`K`	`A`	`LDA`	`B`	`LDB`	`LDC`
1	1	-	1	`gemv`	-	m	n_1	-	$\mathbf{B}$	n_1	$\underline{\mathbf{A}}$	-	-
2	2	$(1,2)$	1	`gemm`	$\mathbf{B}$	n_2	m	n_1	$\underline{\mathbf{A}}$	n_1	$\mathbf{B}$	n_1	m
3	2	$(1,2)$	2	`gemm`	-	m	n_1	n_2	$\mathbf{B}$	n_2	$\underline{\mathbf{A}}$	n_1	n_1
4	2	$(2,1)$	1	`gemm`	-	m	n_2	n_1	$\mathbf{B}$	n_1	$\underline{\mathbf{A}}$	n_2	n_2
5	2	$(2,1)$	2	`gemm`	$\mathbf{B}$	n_1	m	n_2	$\underline{\mathbf{A}}$	n_2	$\mathbf{B}$	n_2	m
6	>2	any	π_1	`gemm`	$\mathbf{B}$	$\bar{n}_q$	m	n_q	$\underline{\mathbf{A}}$	n_q	$\mathbf{B}$	n_q	m
7	>2	any	π_p	`gemm`	-	m	$\bar{n}_q$	n_q	$\mathbf{B}$	n_q	$\underline{\mathbf{A}}$	$\bar{n}_q$	$\bar{n}_q$
8	>2	any	$\pi_2, .., \pi_{p-1}$	`gemm*`	-	m	n_{π_1}	n_q	$\mathbf{B}$	n_q	$\underline{\mathbf{A}}$	w_q	w_q

Table 1. Eight cases with `gemv` and `gemm` for the mode-q tensor-matrix multiplication. Arguments `T`, `M`, `N`, etc. of the BLAS are chosen with respect to the tensor order p, layout $\boldsymbol{\pi}$ and contraction mode q where `T` specifies if $\mathbf{B}$ is transposed. `gemm*` denotes multiple `gemm` calls with different tensor slices. Argument $\bar{n}_q$ for case 6 and 7 is given by $\bar{n}_q = 1/n_q \prod_r^p n_r$. Matrix $\mathbf{B}$ has the row-major format.

$\mathbf{C} = \mathbf{A} \cdot \mathbf{B}^T$ for $q = 2$. Note that the transposition of $\mathbf{B}$ is necessary for the cases 2,5 and independent of the chosen storage format.

Case 6-7 ($p > 2$)*:* If the order of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ is greater than 2 and if the contraction mode q is equal to π_1 (case 6), a single `gemm` with the depicted parameters executes $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}^T$ and computes a tensor-matrix product $\underline{\mathbf{C}} = \underline{\mathbf{A}} \times_{\pi_1} \mathbf{B}$ for any storage layout of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$. Tensors $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are flattened with $\varphi_{2,p}$ to row-major matrices $\mathbf{A}$ and $\mathbf{C}$. Matrix $\mathbf{A}$ has $\bar{n}_{\pi_1} = \bar{n}/n_{\pi_1}$ rows and n_{π_1} columns while matrix $\mathbf{C}$ has the same number of rows and m columns. If $\pi_p = q$ (case 7), Tensors $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are flattened with $\varphi_{1,p-1}$ to column-major matrices $\mathbf{A}$ and $\mathbf{C}$. Matrix $\mathbf{A}$ has n_{π_p} rows and $\bar{n}_{\pi_p} = \bar{n}/n_{\pi_p}$ columns while matrix $\mathbf{C}$ has m rows and the same number of columns. A single `gemm` executes $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ and computes the tensor-matrix product $\underline{\mathbf{C}} = \underline{\mathbf{A}} \times_{\pi_p} \mathbf{B}$ for any storage layout of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$. Note that in all cases no copy operation is performed in order to compute the desired contraction, see subsection 3.

Case 8 ($p > 2$)*:* If the tensor order is greater than 2 with $\pi_1 \neq q$ and $\pi_p \neq q$, the modified baseline algorithm 1 is used to successively call $\bar{n}/(n_q \cdot n_{\pi_1})$ times `gemm` with different tensor slices of $\underline{\mathbf{C}}$ and $\underline{\mathbf{A}}$ in the base case. Each `gemm` computes one slice $\underline{\mathbf{C}}'_{\pi_1,q}$ of the tensor-matrix product $\underline{\mathbf{C}}$ using the corresponding tensor slices $\underline{\mathbf{A}}'_{\pi_1,q}$ and the matrix $\mathbf{B}$. The matrix-matrix product $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ is performed by interpreting both tensor slices as row-major matrices $\mathbf{A}$ and $\mathbf{C}$ which have the dimensions (n_q, n_{π_1}) and (m, n_{π_1}), respectively.

4.4 BLAS-Based Algorithms with Subtensors

Case 8 can be optimized by utilizing larger subtensors instead of tensor slices. This can be done by adding mergeable modes to the slice-matrix multiplication in which the subtensor can be flattened into a matrix without reordering tensor elements. The flattening operation does not copy or reorder elements, see section 3 and lemma 4.1 in [8]. The number of mergeable modes is $\hat{q}-1$ with $\hat{q} = \boldsymbol{\pi}^{-1}(q)$ and the corresponding modes are $\pi_1, \pi_2, \ldots, \pi_{\hat{q}-1}$. Applying flattening $\varphi_{1,q-1}$ and reshaping ρ with $\boldsymbol{\rho} = (2,1)$ on a subtensor of $\underline{\mathbf{A}}$ with dimensions $n_{\pi_1}, \ldots, n_{\pi_{\hat{q}-1}}, n_q$ yields a row-major matrix $\mathbf{A}$ with shape $(n_q, \prod_{r=1}^{\hat{q}-1} n_{\pi_r})$. Analogously, tensor $\underline{\mathbf{C}}$ becomes a row-major matrix with the shape $(m, \prod_{r=1}^{\hat{q}-1} n_{\pi_r})$. This description supports all linear tensor layouts and generalizes lemma 4.2 in [8].

Algorithm 1 needs a minor modification so that `gemm` can be used with flattened subtensors instead of tensor slices. The modified algorithm therefor iterates only over modes larger than $\hat{q}$ in the non-base case and hence omits the first $\hat{q}$ modes $\boldsymbol{\pi}_{1,\hat{q}} = (\pi_1, \ldots, \pi_{\hat{q}})$ with $\pi_{\hat{q}} = q$. The conditions in line 2 and 4 are changed to $1 < r \leq \hat{q}$ and $\hat{q} < r$, respectively. The single indices of the subtensors $\underline{\mathbf{A}}'_{\boldsymbol{\pi}_{1,\hat{q}}}$ and $\underline{\mathbf{C}}'_{\boldsymbol{\pi}_{1,\hat{q}}}$ are given by the loop induction variables that belong to the π_r-th loop with $\hat{q}+1 \leq r \leq p$.

4.5 Parallel BLAS-based Algorithms

The following paragraphs discuss three parallel approaches for the eighth case. Cases 1 to 7 already call a multi-threaded `gemm` and cannot be further optimized.

Sequential Loops and Multithreaded Matrix Multiplication One straight forward approach is to use algorithm 1 as it is and to sequentially call a multi-threaded `gemm` in the base case of the algorithm as described in subsection 4.4. This is beneficial if $q = \pi_{p-1}$, the inner dimensions $n_{\pi_1}, \ldots, n_q$ are large or the outer-most dimension n_{π_p} is smaller than the available processor cores. However, if the above conditions are not met, the processor cores might not be fully utilized where each multi-threaded `gemm` is executed with small subtensors. We will refer to this algorithm version as `<seq-loops,par-gemm>` that is executable with subtensors or tensor slices.

Parallel Loops and Single or Multithreaded Matrix Multiplication A more advanced version of the above algorithm executes a single-threaded `gemm` in parallel including all available (free) modes which depend on the slicing. If subtensors are used, all $\pi_{\hat{q}+1}, \ldots, \pi_p$ modes are free. In case of tensor slices, only π_1 and $\pi_{\hat{q}}$ are free modes. The corresponding maximum degree of parallelism for both cases are $\prod_{r=\hat{q}+1}^{p} n_{\pi_r}$ and $\prod_{r=1}^{p} n_r/(n_{\pi_1} n_{\pi_{\hat{q}}})$, respectively.

Using tensor slices for the multiplication, $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are flattened twice with $\varphi_{\pi_{\hat{q}+1},\pi_p}$ and $\varphi_{\pi_2,\pi_{\hat{q}-1}}$. The resulting tensor is of order 4 with dimensions n_{π_1}, $\hat{n}_{\pi_2}$, n_q, $\hat{n}_{\pi_4}$ where $\hat{n}_{\pi_2} = \prod_{r=2}^{\hat{q}-1} n_{\pi_r}$ and $\hat{n}_{\pi_4} = \prod_{r=\hat{q}+1}^{p} n_{\pi_r}$. In this way the tree-recursion has been transformed in two loops. The outer loop iterates over $\hat{n}_{\pi_4}$ while the inner loop iterates over $\hat{n}_{\pi_2}$ calling `gemm` with slices $\underline{\mathbf{A}}'_{\pi_1,q}$ and $\underline{\mathbf{C}}'_{\pi_1,q}$. Both loops are parallelized using `omp parallel for` together with the `collapse(2)` and the `num_threads` clause which specifies the thread number.

In case of the general subtensor-matrix approach, both tensors are flattened twice with $\varphi_{\pi_{\hat{q}+1},\pi_p}$ and $\varphi_{\pi_1,\pi_{\hat{q}-1}}$. The resulting tensor is of order 3 with dimensions $\hat{n}_{\pi_1}, n_q, \hat{n}_{\pi_4}$ where $\hat{n}_{\pi_1} = \prod_{r=1}^{\hat{q}-1} n_{\pi_r}$ and $\hat{n}_{\pi_4} = \prod_{r=\hat{q}+1}^{p} n_{\pi_r}$. The corresponding algorithm consists of one loops which iterates over $\hat{n}_{\pi_4}$ calling single-threaded gemm with multiple subtensors $\underline{\mathbf{A}}'_{\boldsymbol{\pi}',q}$ and $\underline{\mathbf{C}}'_{\boldsymbol{\pi}',q}$ with $\boldsymbol{\pi}' = (\pi_1, \dots, \pi_{\hat{q}-1})$.

Both algorithm variants will be referred to as <par-loops,seq-gemm> which can be used with subtensors or tensor slices. Note that <seq-loops,par-gemm> and <par-loops,seq-gemm> are opposing versions where either gemm or the free loops are performed in parallel. The all-parallel version <par-loops,par-gemm> executes available loops in parallel where each loop thread executes a multi-threaded gemm with either subtensors or tensor slices.

Multithreaded batched Matrix Multiplication The next version of the base algorithm is a modified version of the general subtensor-matrix approach that calls a single batched gemm for the eighth case. The subtensor dimensions and remaining gemm arguments remain the same. The library implementation is responsible how subtensor-matrix multiplications are executed and if subtensors are further divided into smaller subtensors or tensor slices. This version will be referred to as the <gemm_batch> variant.

5 Experimental Setup

Computing System The experiments have been carried out on an Intel Xeon Gold 6248R processor with a Cascade micro-architecture. The processor consists of 24 cores operating at a base frequency of 3 GHz for non-AVX512 instructions. With 24 cores and a peak AVX-512 boost frequency of 2.5 GHz, the processor achieves a theoretical data throughput of ca. 1.92 double precision Tflops. We measured a peak performance of 1.78 double precision Tflops using the likwid performance tool.

The source code has been compiled with GCC v10.2 using the highest optimization level -O3 and -march=native, -pthread and -fopenmp. Loops within for the eighth case have been parallelized using GCC's OpenMP v4.5 implementation. We have used the GEMV and GEMM implementation of the 2024.0 Intel MKL and its own threading library mkl_intel_thread together with the threading runtime library libiomp5.

If not otherwise mentioned, both tensors $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are stored according to the first-order linear tensor layout with $\boldsymbol{\pi} = (1, \dots, p)$ whereas matrix $\mathbf{B}$ has the row-major storage format. The benchmark results of each function are the average of 10 runs.

Tensor Shapes We have used asymmetrically-shaped and symmetrically-shaped tensors in order to cover many possible use cases. The dimension tuples of both shape types are organized within two three-dimensional arrays with which tensors are initialized. The dimension array for the first shape type contains $720 = 9 \times 8 \times 10$ dimension tuples where the row number is the tensor order ranging from 2 to 10. For each tensor order 8 tensor instances with increasing tensor size is generated. The second set consists of $336 = 6 \times 8 \times 7$ dimensions tuples where the tensor order ranges from 2 to 7 and has 8 dimension tuples for each order. Each tensor dimension within the second set is 2^{12}, 2^8, 2^6, 2^5, 2^4 and 2^3. A detailed explanation of the tensor shape setup is given in [2,3].

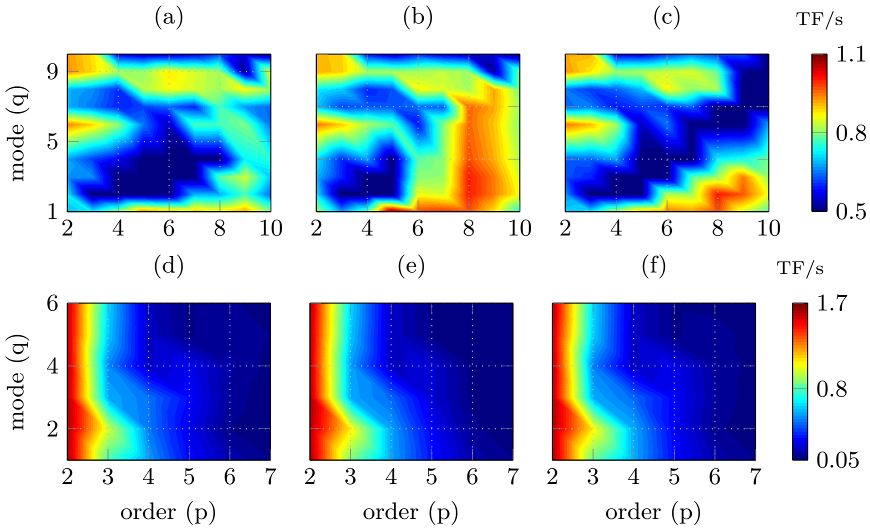

Fig. 1. Performance maps in double-precision Tflops of the proposed algorithms with varying tensor orders p and contraction modes q. Tensors are asymmetrically-shaped on the upper plots and symmetrically-shaped on the lower plots. In (a) and (d) function `<gemm_batch>` is executed, in (b) and (e) `<par-loops,seq-gemm>` with tensor slices, in (c) and (f) `<par-loops,seq-gemm>` with subtensors.

6 Results and Discussion

Slicing Methods The following paragraphs analyze the two proposed slicing methods by benchmarking the functions `<par-loops,seq-gemm>` and `<gemm-batch>` using asymmetrically (top) and symmetrically (bottom) shaped tensors. Fig. 1 contains six contour plots (performance maps) in which `<par-loops,seq-gemm>` either uses subtensors or tensor slices and `<gemm-batch>` loops over subtensors only. Each point within the performance map represents a mean value that has been averaged over tensor sizes for a tensor order[1].

For asymmetrically shaped tensors, function `<par-loops,seq-gemm>` with tensor slices performs on average 18% better than with subtensors. Our function `<par-loops,seq-gemm>` with tensor slices is on average 11% faster than Intel's `gemm_batch` routine and reaches almost 1.1 Tflops for non-edge cases with $q > 2$ and $p > 6$. This suggests that the Intel's implementation does not divide subtensors into smaller blocks.

With symmetrically shaped tensors, `<par-loops,seq-gemm>` with tensor slices performs almost identical as `<gemm-batch>` with 221.52 Gflops and 236.21 Gflops, respectively. Moreover, the slicing method seems to have only little affect on the overall runtime behavior of `<par-loops,seq-gemm>`. In contrast to the perfor-

[1] Note that Fig. 2 suggests that the contraction mode q can be greater than p which is not possible. Our profiling program sets $q = p$ in such cases.

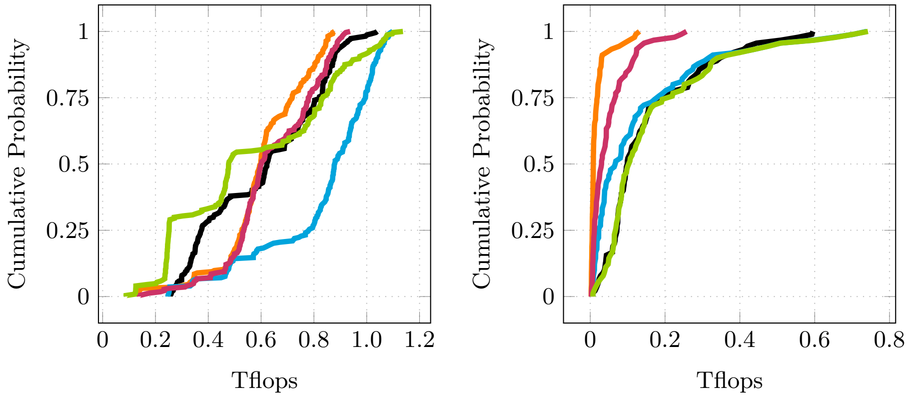

Fig. 2. Cumulative performance distributions of the proposed algorithms for case eight. Each distribution line belongs to one algorithm: `<gemm_batch>` ( ), `<seq-loops,par-gemm>` ( ) and `<par-loops,seq-gemm>` ( ) using tensor slices, `<seq-loops,par-gemm>` ( ) and `<par-loops,seq-gemm>` ( ) using subtensors. Tensors are asymmetrically (left plot) and symmetrically shaped (right plot).

mance maps with asymmetrically shaped tensors, all functions almost reach the attainable peak performance of 1.7 Tflops when $p = 2$. This can by the fact that both dimensions are equal or larger than 4096 enabling `gemm` to operate under optimal conditions.

Parallelization Methods The contour plots in Fig. 1 contain performance data of all cases except for 4 and 5, see Table 1. The effects of the presented slicing and parallelization methods can be better understood if performance data of only the eighth case is examined. Fig. 2 contains cumulative performance distributions of all the proposed algorithms which are generated `gemm` or `gemm_batch` calls within case 8. As the distribution is empirically generated, the probability y of a point (x, y) on a distribution function corresponds to the number of test cases of a particular algorithm that achieves x or less Tflops. For instance, function `<seq-loops,par-gemm>` with subtensors computes the tensor-matrix product with equal to or less than 0.6 Tflops for 50% percent of the test cases using asymmetrically shaped tensor. Consequently, distribution functions with an exponential growth is favorable while logarithmic behavior is less desirable. The test set cardinality for case 8 is 255 for asymmetrically shaped tensors and 91 for symmetrically ones.

In case of asymmetrically shaped tensors, `<par-loops,seq-gemm>` with tensor slices performs best and outperforms `<gemm_batch>`. One unexpected finding is that function `<seq-loops,par-gemm>` with any slicing strategy performs better than `<gemm_batch>` when the tensor order p and contraction mode q satisfy $4 \leq p \leq 7$ and $2 \leq q \leq 4$, respectively. Functions executed with symmetrically shaped tensors reach at most 743 Gflops for the eighth case which is less than half of the attainable peak performance of 1.7 Tflops. This is expected as cases

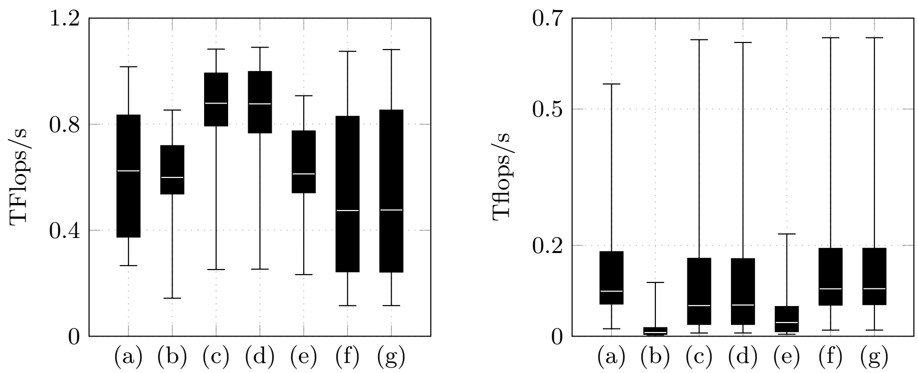

Fig. 3. Box plots visualizing performance statics in double-precision Tflops of a tensor-times-matrix algorithm for linear k-order tensor formats. The algorithm loops over single-threaded `gemm` with tensor slices with asymmetrically-shaped tensors on the left plot and with subtensors with symmetrically-shaped tensors on the right plot. Box plot number k denotes the utilized k-order storage.

2 and 3 are not considered. Functions `<par-loops,seq-gemm>` with subtensors and `<gemm_batch>` have almost the same performance distribution outperforming `<seq-loops,par-gemm>` for almost every test case. Function `<par-loops,seq-gemm>` with tensor slices is on average almost as fast as with subtensors. However, if the tensor order is greater than 3 and the tensor dimensions are less than 64, its running time increases by almost a factor of 2.

These observations suggest to use `<par-loops,seq-gemm>` with tensor slices for common cases in which the leading and contraction dimensions are larger than 64 elements. Subtensors should only be used if the leading dimension n_{π_1} of $\underline{\mathbf{A}}_{\pi_1,q}$ and $\underline{\mathbf{C}}_{\pi_1,q}$ falls below 64. This strategy is different to the one presented in [8] that maximizes the number of modes involved in the matrix multiply. We have also observed no performance improvement if `par-gemm` was used with `par-loops` which is why their distribution functions are not shown in Fig. 2. Moreover, in most cases the `seq-loops` implementations are independent of the tensor shape slower than `par-loops`, even for smaller tensor slices.

Comparison with other Approaches We have compared our best implementation with four libraries that implement the tensor-matrix multiplication using different approaches. Library **tcl** implements the TTGT approach with a high-perform tensor-transpose library **hptt** which is discussed in [15]. **tblis** implements the GETT approach that is akin to Blis' algorithm design for the matrix multiplication [10]. The tensor extension of **eigen** (v3.3.7) is used by the Tensorflow framework. Library **libtorch** (v2.3.0) is the `C++` distribution of PyTorch. **tlib** denotes our library using algorithm `<par-loops,seq-gemm>` that have been presented in the previous paragraphs.

Fig. 2 contains cumulative performance distributions for the complete test sets comparing the performance distribution of our implementation with the pre-

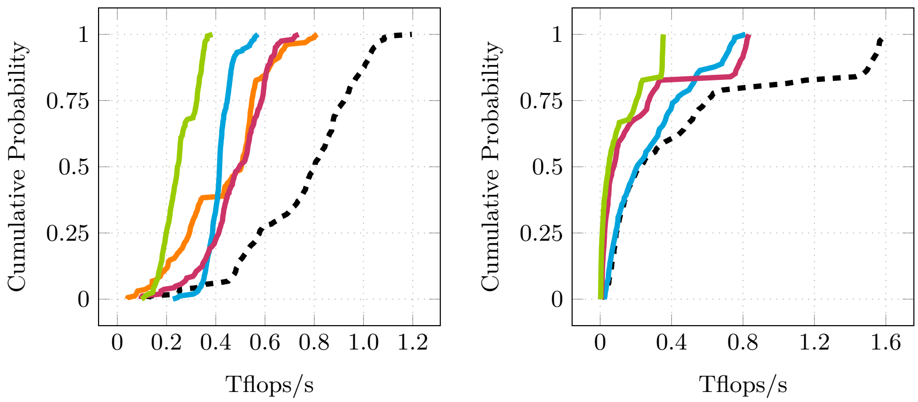

Fig. 4. Cumulative performance distributions of tensor-times-matrix algorithms in double-precision Tflops. Each distribution line belongs to a library: **tlib**[ours] (▪▪▪), **tcl** (▬), **tblis** (▬), **libtorch** (▬), **eigen** (▬). Libraries have been tested with asymmetrically-shaped (left plot) and symmetrically-shaped tensors (right plot).

viously mentioned libraries. Note that we only have used tensor slices for asymmetrically shaped tensors (left plot) and subtensors for symmetrically shaped tensors (right plot). Our implementation with a median performance of 793.75 Gflops outperforms others' for almost every asymmetrically shaped tensor in the test set. The median performances of **tcl**, **tblis**, **libtorch** and **eigen** are 503.61, 415.33, 496.22 and 244.69 Gflops reaching on average 74.11%, 61.14%, 76.68% and 39.34% of **tlib**'s throughputs.

In case of symmetrically shaped tensors the performance distributions of all libraries on the right plot in Fig. 2 are much closer. The median performances of **tlib**, **tblis**, **libtorch** and **eigen** are 228.93, 208.69, 76.46, 46.25 Gflops reaching on average 73.06%, 38.89%, 19.79% of **tlib**'s throughputs[2]. All libraries operate with 801.68 or less Gflops for the cases 2 and 3 which is almost half of **tlib**'s performance with 1579 Gflops. The median performance and the interquartile range of **tblis** and **tlib** for the cases 6 and 7 are almost the same. Their respective median Gflops are 255.23 and 263.94 for the sixth case and 121.17 and 144.27 for the seventh case. This explains the similar performance distributions when their performance is less than 400 Gflops. **Libtorch** and **eigen** compute the tensor-matrix product, in median, with 17.11 and 9.64 Gfops/s, respectively. Our library **tlib** has a median performance of 102.11 Gflops and outperforms **tblis** with 79.35 Gflops for the eighth case.

[2] We were unable to run tcl with our test set containing symmetrically shaped tensors. We suspect a very high memory demand to be the reason.

7 Conclusion and Future Work

We presented efficient layout-oblivious algorithms for the compute-bound tensor-matrix multiplication which is essential for many tensor methods. Our approach is based on the loops-over-`gemm` method and computes the tensor-matrix product in-place without transposing tensors. It applies the flexible approach described in [2] and generalizes the findings on tensor slicing in [8]. The resulting algorithms are able to process dense tensors with arbitrary tensor order, dimensions and with any linear tensor layout all of which can be runtime variable.

Our benchmarks show that tiling the base algorithm into eight different `gemm` cases improves the overall performance. We have demonstrated that algorithms with parallel loops over single-threaded `gemm` calls with tensor slices and subtensors perform best. Interestingly, they outperform a single `gemm_batch` call with subtensors, on average, by 14% in case of asymmetrically shaped tensors and if tensor slices are used. Both version computes the tensor-matrix product on average at least by 14.05% and up to a factor of 3.79 faster than other state-of-the-art implementations.

Summarizing our findings, LOG-based tensor-times-matrix algorithms are able to outperform TTGT-based and GETT-based implementations without sacrificing on flexibility or maintainability. Hence, other actively developed libraries such as LibTorch and Eigen will benefit from implementing the proposed algorithms. Our header-only library provides C++ interfaces and a python module which allows frameworks to easily integrate our library.

In the future, we intend to generalize LOG-based approach for general tensor contractions with the same flexibility that we offered for the tensor-matrix multiplication. We would like to further optimize the tensor-matrix multiplication based on benchmark results of matrix-matrix products which might lead to better runtime results for edge cases.

Source Code Availability Project description and source code can be found at https://github.com/bassoy/ttm. The sequential tensor-matrix multiplication of `TLIB` is part of `uBLAS` and in the official release of `Boost v1.70.0` or later.

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