Design of a high-performance tensor-matrix multiplication with BLAS

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Abstract

The tensor-matrix multiplication is a basic tensor operation required by various tensor methods such as the HOSVD. This paper presents flexible high-performance algorithms that compute the tensor-matrix product according to the Loops-over-GEMM (LoG) approach. Our algorithms are able to process dense tensors with any linear tensor layout, arbitrary tensor order and dimensions all of which can be runtime variable. We discuss two slicing methods with orthogonal parallelization strategies and propose four algorithms that call BLAS with subtensors or tensor slices. We provide a simple heuristic which selects one of the four proposed algorithms at runtime. All algorithms have been evaluated on a large set of tensors with various tensor shapes and linear tensor layouts. In case of large tensor slices, our best-performing algorithm achieves a median performance of 2.47 TFLOPS on an Intel Xeon Gold 5318Y and 2.93 TFLOPS an AMD EPYC 9354. Furthermore, it outperforms batched GEMM implementation of Intel MKL by a factor of 2.57 with large tensor slices. Our runtime tests show that TLIB'S function <combined> is, in median, between 15.38% and 257.58% faster than most state-of-the-art approaches, including actively developed libraries like Libtorch and Eigen. It is on par with TBLIS for many tensor shapes which uses optimized kernels for the TTM computation. This work is an extended version of the article "Fast and Layout-Oblivious Tensor-Matrix Multiplication with BLAS" (Bassoy, 2024)[1].

1 1. Introduction

Tensor computations are found in many scientific fields such as computational neuroscience, pattern recognition, signal processing and data mining [2, 3, 4, 5, 6]. These computations use basic tensor operations as building blocks for decomposing and analyzing multidimensional data which are represented by tensors [7, 8]. Tensor contractions are an important subset of basic operations that need to be fast for efficiently solving tensor methods.

There are three main approaches for implementing ten-11 sor contractions. The Transpose Transpose GEMM Trans-12 pose (TGGT) approach reorganizes tensors in order to 13 perform a tensor contraction using optimized implemen-14 tations of the general matrix multiplication (GEMM) [9, 15 10. GEMM-like Tensor-Tensor multiplication (GETT) 16 method implement macro-kernels that are similar to the 17 ones used in fast GEMM implementations [11, 12]. The 18 third method is the Loops-over-GEMM (LoG) or the BLAS-19 based approach in which Basic Linear Algebra Subpro-20 grams (BLAS) are utilized with multiple tensor slices or 21 subtensors if possible [13, 14, 15, 16]. The BLAS are 22 considered the de facto standard for writing efficient and 23 portable linear algebra software, which is why nearly all ²⁴ processor vendors provide highly optimized BLAS imple-25 mentations. Implementations of the LoG and TTGT ap-26 proaches are in general easier to maintain and faster to 27 port than GETT implementations which might need to

²⁸ adapt vector instructions or blocking parameters accord-²⁹ ing to a processor's microarchitecture.

In this work, we present high-performance algorithms 31 for the tensor-matrix multiplication (TTM) which is used 32 in important numerical methods such as the higher-order 33 singular value decomposition and higher-order orthogonal 34 iteration [17, 8, 7]. TTM is a compute-bound tensor op-35 eration and has the same arithmetic intensity as a matrix-36 matrix multiplication which can almost reach the practical 37 peak performance of a computing machine. To our best 38 knowledge, we are the first to combine the LoG-approach 39 described in [16, 18] for tensor-vector multiplications with 40 the findings on tensor slicing for the tensor-matrix mul-41 tiplication in [14]. Our algorithms support dense tensors 42 with any order, dimensions and any linear tensor layout 43 including the first- and the last-order storage formats for 44 any contraction mode all of which can be runtime variable. 45 Supporting arbitrary tensor layouts enables other frame-46 works non-column-major storage formats to easily inte-47 grate our library without tensor reformatting and unneces-48 sary copy operations¹. Our implementation compute the 49 tensor-matrix product in parallel using efficient GEMM 50 without transposing or flattening tensors. In addition to 51 their high performance, all algorithms are layout-oblivious 52 and provide a sustained performance independent of the 53 tensor layout and without tuning. We provide a single al-54 gorithm that selects one of the proposed algorithms based 55 on a simple heuristic.

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¹For example, Tensorly [19] requires tensors to be stored in the last-order storage format (row-major).

₅₇ less than 150 lines of C++ code where the algorithmic ₁₁₀ plication. Algorithm design and methods for slicing and 58 complexity is reduced by the BLAS implementation and 111 parallel execution are discussed in Section 4. Section 5 59 the corresponding selection of subtensors or tensor slices. 112 describes the test setup. Benchmark results are presented 60 We have provided an open-source C++ implementation of 113 in Section 6. Conclusions are drawn in Section 8. 61 all algorithms and a python interface for convenience.

The analysis in this work quantifies the impact of the 63 tensor layout, the tensor slicing method and parallel exe-64 cution of slice-matrix multiplications with varying contrac-65 tion modes. The runtime measurements of our implemen-66 tations are compared with state-of-the-art approaches dis-67 cussed in [11, 12, 20] including Libtorch and Eigen. While 68 our implementation have been benchmarked with the In-69 tel MKL and AMD AOCL libraries, the user choose other 70 BLAS libraries. In summary, the main findings of our work 71 are:

Given a row-major or column-major input matrix, the tensor-matrix multiplication with tensors of any linear tensor layout can be implemented by an inplace algorithm with 1 GEMV and 7 GEMM instances, supporting all combinations of contraction mode, tensor order and tensor dimensions.

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- The proposed algorithms show a similar performance characteristic across different tensor layouts, provided that the contraction conditions remain the same.
- A simple heuristic is sufficient to select one of the proposed algorithms at runtime, providing a nearoptimal performance for a wide range of tensor shapes. 136
- Our best-performing algorithm is a factor of 2.57 faster than Intel's batched GEMM implementation for large tensor slices.
- Our best-performing algorithm has a median performance speedup between 15.38% and 257.58% compared to other state-of-the art library implementations, including LibTorch and Eigen.

This work is an extended version of the article "Fast 92 and Layout-Oblivious Tensor-Matrix Multiplication with 93 BLAS" [1]. Compared to our previous publication, we have 94 made several significant additions. We conducted runtime 95 tests on a more recent Intel Xeon Gold 5318Y CPU and 96 expanded our study to include AMD's AOCL, running ad-97 ditional benchmarks on an AMD EPYC 9354 CPU. We in-98 corporated a newer version of TBLIS while also testing the 99 TuckerMPI TTM implementation. Furthermore, we ex-100 tended our implementations to support the column-major 101 matrix storage format and benchmarked our algorithms for 102 both row-major and column-major layouts, analyzing the 103 runtime results in detail. Lastly, we introduced a heuristic 104 that enables the use of a single TTM algorithm, ensuring 105 efficiency across different storage formats and a wide range 106 of tensor shapes.

The remainder of the paper is organized as follows. 108 Section 2 presents related work. Section 3 introduces some

Every proposed algorithm can be implemented with 109 notation on tensors and defines the tensor-matrix multi-

114 2. Related Work

Springer et al. [11] present a tensor-contraction gen-116 erator TCCG and the GETT approach for dense tensor 117 contractions that is inspired from the design of a high-118 performance GEMM. Their unified code generator selects 119 implementations from generated GETT, LoG and TTGT 120 candidates. Their findings show that among 48 different 121 contractions 15% of LoG-based implementations are the 122 fastest.

Matthews [12] presents a runtime flexible tensor con-124 traction library that uses GETT approach as well. He de-125 scribes block-scatter-matrix algorithm which uses a special 126 layout for the tensor contraction. The proposed algorithm 127 yields results that feature a similar runtime behavior to 128 those presented in [11].

Li et al. [14] introduce InTensLi, a framework that 130 generates in-place tensor-matrix multiplication according 131 to the LoG approach. The authors discusses optimization 132 and tuning techniques for slicing and parallelizing the op-133 eration. With optimized tuning parameters, they report 134 a speedup of up to 4x over the TTGT-based MATLAB 135 tensor toolbox library discussed in [9].

Bassoy [16] presents LoG-based algorithms that com-137 pute the tensor-vector product. They support dense ten-138 sors with linear tensor layouts, arbitrary dimensions and 139 tensor order. The presented approach contains eight cases 140 calling GEMV and DOT. He reports average speedups of 141 6.1x and 4.0x compared to implementations that use the 142 TTGT and GETT approach, respectively.

Pawlowski et al. [18] propose morton-ordered blocked 144 layout for a mode-oblivious performance of the tensor-145 vector multiplication. Their algorithm iterate over blocked 146 tensors and perform tensor-vector multiplications on blocked 147 tensors. They are able to achieve high performance and 148 mode-oblivious computations.

In [21] the authors present a C++ software package 150 (TuckerMPI) for large-scale data compression using ten-151 sor tucker decomposition. The library provides a parallel 152 C++ function of the latter containing distributed func-153 tions with MPI for the Gram computation and tensor-154 matrix multiplication. Th latter invokes a local version 155 that contains a multi-threaded gemm computing the tensor-156 matrix product with submatrices according to the LoG 157 approach. The presented local TTM corresponds to our 158 <par-gemm, subtensor> version.

159 3. Background

160 3.1. Tensor Notation

An order-p tensor is a p-dimensional array where ten-162 sor elements are contiguously stored in memory[22, 7]. 163 We write a, \mathbf{a} , \mathbf{A} and $\underline{\mathbf{A}}$ in order to denote scalars, vec-165 we assume $\underline{\mathbf{A}}$ to have order p>2. The p-tuple $\mathbf{n}=$ (n_1, n_2, \ldots, n_p) will be referred to as the shape or dimen-167 sion tuple of a tensor where $n_r > 1$. 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 $\mathbf{i}=(i_1,i_2,\ldots,i_p)$ is a multi-index. For con-170 venience, we will also use square brackets to concatenate 171 index tuples such that $[\mathbf{i}, \mathbf{j}] = (i_1, i_2, \dots, i_r, j_1, j_2, \dots, j_q)$ where **i** and **j** are multi-indices of length r and q, respec-173 tively.

174 3.2. Tensor-Matrix Multiplication (TTM)

176 ([$\mathbf{n}_1, n_q, \mathbf{n}_2$]) and $\mathbf{n}_c = ([\mathbf{n}_1, m, \mathbf{n}_2])$ where $\mathbf{n}_1 = (n_1, n_2, n_2)$ 177 ..., n_{q-1}) and $\mathbf{n}_2 = (n_{q+1}, n_{q+2}, \dots, n_p)$. Let **B** be a ma-178 trix of shape $\mathbf{n}_b=(m,n_q)$. A q-mode tensor-matrix prod-228 fined as $\hat{q}=\pi^{-1}(q)$. Given a layout tuple π with p

$$\underline{\mathbf{C}}([\mathbf{i}_1, j, \mathbf{i}_2]) = \sum_{i_n=1}^{n_q} \underline{\mathbf{A}}([\mathbf{i}_1, i_q, \mathbf{i}_2]) \cdot \mathbf{B}(j, i_q)$$
(1)

with $\mathbf{i}_1 = (i_1, \dots, i_{q-1})$, $\mathbf{i}_2 = (i_{q+1}, \dots, i_p)$ where $1 \leq i_r \leq n_r$ and $1 \leq j \leq m$ [14, 8]. The mode q is called the 183 contraction mode with $1 \leq q \leq p$. TTM generalizes the $_{184}$ computational aspect of the two-dimensional case $\mathbf{C} =$ 185 $\mathbf{B} \cdot \mathbf{A}$ if p = 2 and q = 1. Its arithmetic intensity is $_{186}$ equal to that of a matrix-matrix multiplication which is 187 compute-bound for large dense matrices.

In the following, we assume that the tensors A and C 189 have the same tensor layout π . Elements of matrix **B** can 190 be stored either in the column-major or row-major format. 191 With i_q iterating over the second mode of **B**, TTM is also $_{192}$ referred to as the q-mode product which is a building block 193 for tensor methods such as the higher-order orthogonal 194 iteration or the higher-order singular value decomposition 195 [8]. Please note that the following method can be applied, 196 if indices j and i_q of matrix **B** are swapped.

197 3.3. Subtensors

A subtensor references elements of a tensor \mathbf{A} and is 199 denoted by \mathbf{A}' . It is specified by a selection grid that con- $_{200}$ sists of p index ranges. In this work, an index range of a $_{201}$ given mode r shall either contain all indices of the mode 202 r or a single index i_r of that mode where $1 \leq r \leq p$. Sub- $_{\rm 203}$ tensor dimensions n_r' are either n_r if the full index range $_{\rm 204}$ or 1 if a a single index for mode r is used. Subtensors are 205 annotated by their non-unit modes such as $\underline{\mathbf{A}}'_{u,v,w}$ where $n_u > 1, n_v > 1 \text{ and } n_w > 1 \text{ for } 1 \le u \ne v \ne w \le p.$ The 207 remaining single indices of a selection grid can be inferred

208 by the loop induction variables of an algorithm. The num-209 ber of non-unit modes determine the order p' of subtensor where $1 \leq p' < p$. In the above example, the subten- $\underline{\mathbf{A}}'_{u,v,w}$ has three non-unit modes and is thus of order 212 3. For convenience, we might also use an dimension tuple 213 **m** of length p' with $\mathbf{m} = (m_1, m_2, \dots, m_{p'})$ to specify a 164 tors, matrices and tensors. If not otherwise mentioned, 214 mode-p' subtensor $\underline{\mathbf{A}}'_{\mathbf{m}}$. An order-2 subtensor of $\underline{\mathbf{A}}'$ is a 215 tensor slice $\mathbf{A}'_{u,v}$ and an order-1 subtensor of $\underline{\mathbf{A}}'$ is a fiber

217 3.4. Linear Tensor Layouts

We use a layout tuple $\pi \in \mathbb{N}^p$ to encode all linear 219 tensor layouts including the first-order or last-order lay-220 out. They contain permuted tensor modes whose priority $_{221}$ is given by their index. For instance, the general k-order $_{222}$ tensor layout for an order-p tensor is given by the layout 223 tuple $\boldsymbol{\pi}$ with $\pi_r = k - r + 1$ for $1 < r \le k$ and r for $224 k < r \le p$. The first- and last-order storage formats are Let $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ be order-p tensors with shapes $\mathbf{n}_a = 225$ given by $\boldsymbol{\pi}_F = (1, 2, \dots, p)$ and $\boldsymbol{\pi}_L = (p, p-1, \dots, 1)$. 226 An inverse layout tuple π^{-1} is defined by $\pi^{-1}(\pi(k)) = k$. 227 Given the contraction mode q with $1 \leq q \leq p$, \hat{q} is deuct is denoted by $\underline{\mathbf{C}} = \underline{\mathbf{A}} \times_q \mathbf{B}$. An element of $\underline{\mathbf{C}}$ is defined 229 modes, the π_r -th element of a stride tuple \mathbf{w} is given by 180 by 230 $w_{\pi_r} = \prod_{k=1}^{r-1} n_{\pi_k}$ for $1 < r \le p$ and $w_{\pi_1} = 1$. Tensor elements of the π_1 -th mode are contiguously stored in mem-232 ory. Their location is given by the layout function $\lambda_{\mathbf{w}}$ ²³³ which maps a multi-index **i** to a scalar index such that ²³⁴ $\lambda_{\mathbf{w}}(\mathbf{i}) = \sum_{r=1}^{p} w_r(i_r - 1)$ [23].

235 3.5. Reshaping

The reshape operation defines a non-modifying refor-237 matting transformation of dense tensors with contiguously 238 stored elements and linear tensor layouts. It transforms 239 an order-p tensor $\underline{\mathbf{A}}$ with a shape \mathbf{n} and layout $\boldsymbol{\pi}$ tu-₂₄₀ ple to an order-p' view $\underline{\mathbf{B}}$ with a shape \mathbf{m} and layout ₂₄₁ $\boldsymbol{\tau}$ tuple of length p' with p' = p - v + u and $1 \leq u < v$ $v \leq p$. Given a layout tuple π of $\underline{\mathbf{A}}$ and contiguous 243 modes $\hat{\boldsymbol{\pi}} = (\pi_u, \pi_{u+1}, \dots, \pi_v)$ of $\boldsymbol{\pi}$, reshape function $\varphi_{u,v}$ 244 is defined as follows. With $j_k=0$ if $k\leq u$ and $j_k=0$ $_{245}v - u$ if k > u where $1 \le k \le p'$, the resulting lay-²⁴⁶ out tuple $oldsymbol{ au}=(au_1,\ldots, au_{p'})$ of $oldsymbol{\mathbf{B}}$ is then given by $au_u=$ $au_{u,v}$ and $au_k = \pi_{k+j_k} - s_k$ for $k \neq u$ with $s_k = \pi_{u,v}$ $_{248} |\{\pi_i \mid \pi_{k+j_k} > \pi_i \wedge \pi_i \neq \min(\hat{\boldsymbol{\pi}}) \wedge u \leq i \leq p\}|.$ Elements of ₂₄₉ the shape tuple **m** are defined by $m_{\tau_u} = \prod_{k=u}^v n_{\pi_k}$ and ₂₅₀ $m_{\tau_k} = n_{\pi_{k+j}}$ for $k \neq u$. Note that reshaping is not related 251 to tensor unfolding or the flattening operations which re-²⁵² arrange tensors by copying tensor elements [8, p.459].

253 4. Algorithm Design

254 4.1. Baseline Algorithm with Contiguous Memory Access The tensor-matrix multiplication (TTM) in equation 256 1 can be implemented with a single algorithm that uses 257 nested recursion. Similar the algorithm design presented 258 in [23], it consists of if statements with recursive calls and 259 an else branch which is the base case of the algorithm.

```
\mathtt{ttm}(\underline{\mathbf{A}},\mathbf{B},\underline{\mathbf{C}},\mathbf{n},\boldsymbol{\pi},\mathbf{i},m,q,\hat{q},r)
 1
 2
                  if r = \hat{a} then
                           \mathsf{ttm}(\underline{\mathbf{A}}, \mathbf{B}, \underline{\mathbf{C}}, \mathbf{n}, \boldsymbol{\pi}, \mathbf{i}, m, q, \hat{q}, r-1)
 3
                  else if r > 1 then
 4
                             for i_{\pi_r} \leftarrow 1 to n_{\pi_r} do
 5
                                       ttm(\underline{\mathbf{A}}, \mathbf{B}, \underline{\mathbf{C}}, \mathbf{n}, \boldsymbol{\pi}, \mathbf{i}, m, q, \hat{q}, r-1)
  6
                             for j \leftarrow 1 to m do
 8
                                        for i_q \leftarrow 1 to n_q do
 9
10
                                                   for i_{\pi_1} \leftarrow 1 to n_{\pi_1} do
                                                       \underline{\mathbf{C}}([\mathbf{i}_1, j, \mathbf{i}_2]) + \underline{\mathbf{A}}([\mathbf{i}_1, i_q, \mathbf{i}_2]) \cdot \mathbf{B}(j, i_q)
```

Algorithm 1: Modified baseline algorithm for TTM with contiguous memory access. The tensor order p must be greater than 1 and the contraction mode q must satisfy $1 \le q \le p$ and $\pi_1 \ne q$. The initial call must happen with r = p where **n** is the shape tuple of $\underline{\mathbf{A}}$ and m is the q-th dimension of $\underline{\mathbf{C}}$. Iteration along mode q with $\hat{q} = \pi_q^{-1}$ is moved into the inner-most recursion

260 A naive implementation recursively selects fibers of the 261 input and output tensor for the base case that computes 262 a fiber-matrix product. The outer loop iterates over the 263 dimension m and selects an element of $\underline{\mathbf{C}}$'s fiber and a row $_{264}$ of **B**. The inner loop then iterates over dimension n_q and 265 computes the inner product of a fiber of $\underline{\mathbf{A}}$ and the row $_{266}$ B. In this case, elements of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are accessed non-267 contiguously whenever $\pi_1 \neq q$ and matrix **B** is accessed $_{268}$ only with unit strides if it elements are stored contiguously 269 along its rows.

A better approach is illustrated in algorithm 1 where $_{271}$ the loop order is adjusted to the tensor layout π and mem-₂₇₂ ory is accessed contiguously for $\pi_1 \neq q$ and p > 1. The ₃₂₇ major order, parameter CBLAS_ORDER of function gemm is 273 algorithm takes the input order-p tensor A, input matrix 328 set to CblasRowMajor (rm) and CblasColMajor (cm) other- \mathbf{B} , order-p output tensor \mathbf{C} , the shape tuple \mathbf{n} of \mathbf{A} , the $_{275}$ layout tuple π of both tensors, an index tuple π of length $_{276}$ p, the first dimension m of **B**, the contraction mode q 277 with $1 \le q \le p$ and $\hat{q} = \pi^{-1}(q)$. The algorithm is initially 278 called with $\mathbf{i} = \mathbf{0}$ and r = p. With increasing recursion $_{279}$ level and decreasing r, the algorithm increments indices with smaller strides as $w_{\pi_r} \leq w_{\pi_{r+1}}$. This is accomplished 335 by a matrix-matrix multiplication where the input tensor 281 in line 5 which uses the layout tuple π to select a multi-282 index element i_{π_r} and to increment it with the correspond-283 ing stride w_{π_r} . The two if statements in line number 2 284 and 4 allow the loops over modes q and π_1 to be placed 285 into the base case in which a slice-matrix multiplication 286 is performed. The inner-most loop of the base case in-₂₈₇ crements i_{π_1} with a unit stride and contiguously accesses 288 tensor elements of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$. The second loop increments 289 i_q with which elements of **B** are contiguously accessed if $_{290}$ B is stored in the row-major format. The third loop in-291 crements j and could be placed as the second loop if **B** is 292 stored in the column-major format.

While spatial data locality is improved by adjusting ²⁹⁴ the loop ordering, slices $\underline{\mathbf{A}}'_{\pi_1,q}$, fibers $\underline{\mathbf{C}}'_{\pi_1}$ and elements $\underline{\mathbf{B}}(j,i_q)$ are accessed $m,\ n_q$ and n_{π_1} times, respectively. ²⁹⁶ The specified fiber of $\underline{\mathbf{C}}$ might fit into first or second level

297 cache, slice elements of $\underline{\mathbf{A}}$ are unlikely to fit in the local 298 caches if the slice size $n_{\pi_1} \times n_q$ is large, leading to higher 299 cache misses and suboptimal performance. Instead of at-300 tempting to improve the temporal data locality, we make 301 use of existing high-performance BLAS implementations 302 for the base case. The following subsection explains this 303 approach.

304 4.2. BLAS-based Algorithms with Tensor Slices

The following approach utilizes the CBLAS gemm func-306 tion in the base case of Algorithm 1 in order to perform 307 fast slice-matrix multiplications². Function gemm denotes 308 a general matrix-matrix multiplication which is defined as 309 C:=a*op(A)*op(B)+b*C where a and b are scalars, A, B and 310 C are matrices, op(A) is an M-by-K matrix, op(B) is a K-by-N 311 matrix and C is an N-by-N matrix. Function op(x) either 312 transposes the corresponding matrix x such that op(x)=x, 313 or not op(x)=x. The CBLAS interface also allows users to 314 specify matrix's leading dimension by providing the LDA, 315 LDB and LDC parameters. A leading dimension specifies 316 the number of elements that is required for iterating over 317 the non-contiguous matrix dimension. The leading dimen-318 sion can be used to perform a matrix multiplication with 319 submatrices or even fibers within submatrices. The lead-320 ing dimension parameter is necessary for the BLAS-based 321 TTM.

The eighth TTM case in Table 1 contains all argu-323 ments that are necessary to perform a CBLAS gemm in 324 the base case of Algorithm 1. The arguments of gemm are set according to the tensor order p, tensor layout π and $_{326}$ contraction mode q. If the input matrix **B** has the row-329 wise. The eighth case will be denoted as the general case 330 in which function gemm is called multiple times with dif-331 ferent tensor slices. Next to the eighth TTM case, there 332 are seven corner cases where a single gemv or gemm call suf-333 fices to compute the tensor-matrix product. For instance 334 if $\pi_1 = q$, the tensor-matrix product can be computed 336 A can be reshaped and interpreted as a matrix without 337 any copy operation. Note that Table 1 supports all linear $_{338}$ tensor layouts of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ with no limitations on tensor 339 order and contraction mode. The following subsection de- $_{340}$ scribes all eight TTM cases when the input matrix ${f B}$ has 341 the row-major ordering.

342 4.2.1. Row-Major Matrix Multiplication

The following paragraphs introduce all TTM cases that 344 are listed in Table 1.

Case 1: If p = 1, The tensor-vector product $\mathbf{A} \times_1 \mathbf{B}$ can $_{346}$ be computed with a gemv operation where **A** is an order-1 347 tensor **a** of length n_1 such that $\mathbf{a}^T \cdot \mathbf{B}$.

²CBLAS denotes the C interface to the BLAS.

Case	Order p	Layout $\pi_{\underline{\mathbf{A}},\underline{\mathbf{C}}}$	Layout $\pi_{\mathbf{B}}$	$\mathrm{Mode}\; q$	Routine	Т	М	N	K	A	LDA	В	LDB	LDC
1	1	-	rm/cm	1	gemv	-	m	n_1	-	В	n_1	<u>A</u>	-	-
2	2	cm	rm	1	gemm	В	n_2	m	n_1	<u>A</u>	n_1	В	n_1	\overline{m}
	2	cm	cm	1	gemm	-	m	n_2	n_1	\mathbf{B}	m	$\underline{\mathbf{A}}$	n_1	m
3	2	cm	rm	2	gemm	-	m	n_1	n_2	\mathbf{B}	n_2	$\underline{\mathbf{A}}$	n_1	n_1
	2	cm	cm	2	gemm	\mathbf{B}	n_1	m	n_2	$\underline{\mathbf{A}}$	n_1	\mathbf{B}	m	n_1
4	2	rm	rm	1	gemm	-	m	n_2	n_1	\mathbf{B}	n_1	$\underline{\mathbf{A}}$	n_2	n_2
	2	rm	cm	1	gemm	\mathbf{B}	n_2	m	n_1	$\underline{\mathbf{A}}$	n_2	$\overline{\mathbf{B}}$	m	n_2
5	2	rm	rm	2	gemm	\mathbf{B}	n_1	m	n_2	$\overline{\mathbf{A}}$	n_2	\mathbf{B}	n_2	m
	2	rm	cm	2	gemm	-	m	n_1	n_2	$\overline{\mathbf{B}}$	m	$\underline{\mathbf{A}}$	n_2	m
6	> 2	any	rm	π_1	gemm	В	\bar{n}_q	m	n_q	<u>A</u>	n_q	В	n_q	\overline{m}
	> 2	any	cm	π_1	gemm	-	m	\bar{n}_q	n_q	\mathbf{B}	m	$\underline{\mathbf{A}}$	n_q	m
7	> 2	any	rm	π_p	gemm	-	m	\bar{n}_q	n_q	\mathbf{B}	n_q	$\underline{\mathbf{A}}$	\bar{n}_q	\bar{n}_q
	> 2	any	cm	π_p	gemm	\mathbf{B}	\bar{n}_q	m	n_q	$\underline{\mathbf{A}}$	\bar{n}_q	$\overline{\mathbf{B}}$	m	\bar{n}_q
8	> 2	any	rm	$\pi_2,, \pi_{p-1}$	gemm*	-	m	n_{π_1}	n_q	В	n_q	<u>A</u>	w_q	w_q
	> 2	any	cm	$\pi_2,, \pi_{p-1}$	gemm*	\mathbf{B}	n_{π_1}	m	n_q	<u>A</u>	w_q	\mathbf{B}	m	w_q

Table 1: Eight TTM cases implementing the mode-q TTM with the gemm and gemv CBLAS functions. Arguments of gemv and gemm (T, M, N, dots) are chosen with respect to the tensor order p, layout π of $\underline{\mathbf{A}}$, $\underline{\mathbf{B}}$, $\underline{\mathbf{C}}$ and contraction mode q where T specifies if $\underline{\mathbf{B}}$ is transposed. Function gemm* with a star denotes multiple gemm calls with different tensor slices. Argument \bar{n}_q for case 6 and 7 is defined as $\bar{n}_q = (\prod_r^p n_r)/n_q$. Input matrix **B** is either stored in the column-major or row-major format. The storage format flag set for gemm and gemv is determined by the element ordering of B.

Case 2-5: If p=2, $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are order-2 tensors with 382 4.2.2. Column-Major Matrix Multiplication $_{349}$ dimensions n_1 and n_2 . In this case the tensor-matrix prod- $_{383}$ $_{350}$ uct can be computed with a single gemm. If ${\bf A}$ and ${\bf C}$ have $_{384}$ column-major version of gemm when the input matrix ${\bf B}$ is $_{351}$ the column-major format with $\pi=(1,2),$ gemm either ex- $_{385}$ stored in column-major order. Although the number of 352 ecutes $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}^T$ for q = 1 or $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ for q = 2. 386 gemm cases remains the same, the gemm arguments must be $_{353}$ Both matrices can be interpreted C and A as matrices in $_{387}$ rearranged. The argument arrangement for the column-354 row-major format although both are stored column-wise. 388 major version can be derived from the row-major version 355 If **A** and **C** have the row-major format with $\pi = (2,1)$, 389 that is provided in table 1. 356 gemm either executes $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ for q = 1 or $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}^T$ for 390 $_{357}$ q=2. The transposition of ${f B}$ is necessary for the TTM $_{391}$ swapped and the transposition flag for matrix ${f B}$ is toggled. 358 cases 2 and 5 which is independent of the chosen layout. 360 gemm with the corresponding arguments executes $\mathbf{C} = \mathbf{A} \cdot \,\,_{394}$ dimension of B. ₃₆₁ \mathbf{B}^T and computes a tensor-matrix product $\mathbf{C} = \mathbf{A} \times_{\pi_1} \mathbf{B}$. ₃₉₅ ₃₆₂ Tensors $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are reshaped with $\varphi_{2,p}$ to row-major ₃₉₆ in Table 1 where tensor $\underline{\mathbf{A}}$ and matrix \mathbf{B} are passed to matrices **A** and **C**. Matrix **A** has $\bar{n}_{\pi_1} = \bar{n}/n_{\pi_1}$ rows and $\bar{n}_{\pi_1} = \bar{n}/n_{\pi_1}$ $_{364}$ n_{π_1} columns while matrix ${f C}$ has the same number of rows $_{398}$ tained when tensor ${f A}$ and matrix ${f B}$ are passed to ${f A}$ and and m columns. If $\pi_p = q$ (case 7), $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ are reshaped 399 B where the transpose flag for \mathbf{B} is set and the remaining 366 with $\varphi_{1,p-1}$ to column-major matrices **A** and **C**. Matrix

371 copy operations, see subsection 3.5. Case 8 (p > 2): If the tensor order is greater than 2 373 with $\pi_1 \neq q$ and $\pi_p \neq q$, the modified baseline algorithm $_{\mbox{\scriptsize 374}}$ 1 is used to successively call $\bar{n}/(n_q\cdot n_{\pi_1})$ times gemm with $_{375}$ different tensor slices of $\underline{\mathbf{C}}$ and $\underline{\mathbf{A}}.$ Each gemm computes one slice $\underline{\mathbf{C}}'_{\pi_1,q}$ of the tensor-matrix product $\underline{\mathbf{C}}$ using the $_{379}$ preting both tensor slices as row-major matrices ${\bf A}$ and ${\bf C}$ 380 which have the dimensions (n_q, n_{π_1}) and (m, n_{π_1}) , respec-381 tively.

367 **A** has n_{π_p} rows and $\bar{n}_{\pi_p} = \bar{n}/n_{\pi_p}$ columns while **C** has $_{368}\;m$ rows and the same number of columns. In this case, a

369 single gemm executes $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ and computes $\mathbf{C} = \mathbf{A} \times_{\pi_n} \mathbf{B}$.

370 Noticeably, the desired contraction are performed without

The tensor-matrix multiplication is performed with the

The CBLAS arguments of M and N, as well as A and B is 392 Also, the leading dimension argument of A is adjusted to Case 6-7: If p > 2 and if $q = \pi_1(\text{case } 6)$, a single 393 LDB or LDA. The only new argument is the new leading

> Given case 4 with the row-major matrix multiplication 400 dimensions are adjusted accordingly.

401 4.2.3. Matrix Multiplication Variations

The column-major and row-major versions of gemm can 403 be used interchangeably by adapting the storage format. 404 This means that a gemm operation for column-major ma-405 trices can compute the same matrix product as one for 406 row-major matrices, provided that the arguments are re-407 arranged accordingly. While the argument rearrangement $_{408}$ is similar, the arguments associated with the matrices A 409 and B must be interchanged. Specifically, LDA and LDB as orresponding tensor slices $\underline{\mathbf{A}}'_{\pi_1,q}$ and the matrix \mathbf{B} . The understand the matrix \mathbf{B} and \mathbf{M} are swapped along with the corresponding matrix-matrix product $\mathbf{C} = \mathbf{B} \cdot \mathbf{A}$ is performed by inter-understanding must 412 be set for A or B in the new format if B or A is transposed 413 in the original version.

> For instance, the column-major matrix multiplication 415 in case 4 of table 1 requires the arguments of A and B to

416 be tensor $\underline{\mathbf{A}}$ and matrix \mathbf{B} with \mathbf{B} being transposed. The 417 arguments of an equivalent row-major multiplication for \mathbf{A} , 418 B, M, N, LDA, LDB and T are then initialized with \mathbf{B} , $\underline{\mathbf{A}}$, m, 419 n_2 , m, n_2 and \mathbf{B} .

Another possible matrix multiplication variant with $_{421}$ the same product is computed when, instead of $\bf B$, ten- $_{422}$ sors $\bf \underline{A}$ and $\bf \underline{C}$ with adjusted arguments are transposed. We assume that such reformulations of the matrix multi- $_{424}$ plication do not outperform the variants shown in Table $_{425}$ 1, as we expect BLAS libraries to have optimal blocking $_{426}$ and multiplication strategies.

427 4.3. Matrix Multiplication with Subtensors

Algorithm 1 can be slightly modified in order to call gemm with reshaped order- \hat{q} subtensors that correspond to larger tensor slices. Given the contraction mode q with 1 < q < p, the maximum number of additionally fusible modes is $\hat{q} - 1$ with $\hat{q} = \pi^{-1}(q)$ where π^{-1} is the inverse layout tuple. The corresponding fusible modes are there-

The non-base case of the modified algorithm only iteradase ates over dimensions that have indices larger than \hat{q} and thus omitting the first \hat{q} modes. The conditions in line 2 and 4 are changed to $1 < r \leq \hat{q}$ and $\hat{q} < r$, respectable tively. Thus, loop indices belonging to the outer π_r -th doop with $\hat{q}+1 \leq r \leq p$ define the order- \hat{q} subtensors $\underline{\mathbf{A}}'_{\pi'}$ and $\underline{\mathbf{C}}'_{\pi'}$ of $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ with $\pi' = (\pi_1, \dots, \pi_{\hat{q}-1}, q)$. Reshaping the subtensors $\underline{\mathbf{A}}'_{\pi'}$ and $\underline{\mathbf{C}}'_{\pi'}$ with $\varphi_{1,\hat{q}-1}$ for the modes dimension π_q or with the fused dimension slices with dimension n_q or with m with the fused dimension $\bar{n}_q = \prod_{r=1}^{\hat{q}-1} n_{\pi_r}$ and $\bar{n}_q = w_q$. Both tensor slices can be interpreted either as row-major or column-major matrices with shapes (n_q, \bar{n}_q) or (w_q, \bar{n}_q) and in case of $\underline{\mathbf{A}}$ and (m, \bar{n}_q) or (\bar{n}_q, m) in case of $\underline{\mathbf{C}}$, respectable tively.

The gemm function in the base case is called with al- most identical arguments except for the parameter M or N which is set to \bar{n}_q for a column-major or row-major multiplication, respectively. Note that neither the selection of the subtensor nor the reshaping operation copy tensor elements. This description supports all linear tensor layouts and generalizes lemma 4.2 in [14] without copying tensor elements, see section 3.5. The division in large subtensors has also been described in [21] for tensors with a first-order layout.

459 4.4. Parallel BLAS-based Algorithms

Most BLAS libraries provide an option to change the number of threads. Hence, functions such as gemm and gemv can be run either using a single or multiple threads. The TTM cases one to seven contain a single BLAS call which why we set the number of threads to the number of available cores. The following subsections discuss parallel versions for the eighth case in which the outer loops of algorithm 1 and the gemm function inside the base case can be run in parallel. Note that the parallelization strategies can be combined with the aforementioned slicing methods.

Algorithm 2: Function ttm<par-loop><slice> is an optimized version of Algorithm 1. The reshape function transforms the order-p tensors $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ with layout tuple π and their respective dimension tuples \mathbf{n} and \mathbf{m} into order-4 tensors $\underline{\mathbf{A}}'$ and $\underline{\mathbf{C}}'$ with layout tuple π' and their respective dimension tuples \mathbf{n}' and \mathbf{m}' where $\mathbf{n}' = (n_{\pi_1}, \hat{n}_{\pi_2}, n_q, \hat{n}_{\pi_4})$ and $m_3' = m$ and $n_k' = m_k'$ for $k \neq 3$. Each thread calls multiple single-threaded gemm functions each of which executes a slice-matrix multiplication with the order-2 tensor slices $\underline{\mathbf{A}}'_{ij}$ and $\underline{\mathbf{C}}'_{ij}$. Matrix $\underline{\mathbf{B}}$ has the row-major storage format.

470 4.4.1. Sequential Loops and Parallel Matrix Multiplication Algorithm 1 is run for the eighth case and does not 472 need to be modified except for enabling gemm to run multi-473 threaded in the base case. This type of parallelization 474 strategy might be beneficial with order- \hat{q} subtensors where 475 the contraction mode satisfies $q = \pi_{p-1}$, the inner dimen-476 sions $n_{\pi_1},\ldots,n_{\hat{q}}$ are large and the outer-most dimension 477 n_{π_p} is smaller than the available processor cores. For 478 instance, given a first-order storage format and the con-479 traction mode q with q=p-1 and $n_p=2$, the di-480 mensions of reshaped order-q subtensors are $\prod_{r=1}^{p-2} n_r$ and 481 n_{p-1} . This allows gemm to perform with large dimensions 482 using multiple threads increasing the likelihood to reach 483 a high throughput. However, if the above conditions are 484 not met, a multi-threaded gemm operates on small tensor 485 slices which might lead to an suboptimal utilization of the 486 available cores. This algorithm version will be referred to 487 as <par-gemm>. Depending on the subtensor shape, we will 488 either add <slice> for order-2 subtensors or <subtensor> 489 for order- \hat{q} subtensors with $\hat{q} = \pi_q^{-1}$.

⁴⁹⁰ 4.4.2. Parallel Loops and Sequential Matrix Multiplication
⁴⁹¹ Instead of sequentially calling multi-threaded gemm, it is
⁴⁹² also possible to call single-threaded gemms in parallel. Sim⁴⁹³ ilar to the previous approach, the matrix multiplication
⁴⁹⁴ can be performed with tensor slices or order- \hat{q} subtensors.

495 Matrix Multiplication with Tensor Slices. Algorithm 2 with 496 function ttm<par-loop><slice> executes a single-threaded 497 gemm with tensor slices in parallel using all modes except 498 π_1 and $\pi_{\hat{q}}$. The first statement of the algorithm calls 499 the reshape function which transforms tensors $\underline{\mathbf{A}}$ and $\underline{\mathbf{C}}$ 500 without copying elements by calling the reshaping oper-501 ation $\varphi_{\pi_{\hat{q}+1},\pi_p}$ and $\varphi_{\pi_2,\pi_{\hat{q}-1}}$. The resulting tensors $\underline{\mathbf{A}}'$ 502 and $\underline{\mathbf{C}}'$ are of order 4. Tensor $\underline{\mathbf{A}}'$ has the shape $\mathbf{n}' = 503 (n_{\pi_1}, \hat{n}_{\pi_2}, n_q, \hat{n}_{\pi_4})$ with the dimensions $\hat{n}_{\pi_2} = \prod_{r=2}^{\hat{q}-1} n_{\pi_r}$ 504 and $\hat{n}_{\pi_4} = \prod_{r=\hat{q}+1}^p n_{\pi_r}$. Tensor $\underline{\mathbf{C}}'$ has the same shape as 505 $\underline{\mathbf{A}}'$ with dimensions $m'_r = n'_r$ except for the third dimensons sion which is given by $m_3 = m$.

The following two parallel for loops iterate over all free modes. The outer loop iterates over $n_4' = \hat{n}_{\pi_4}$ while

 $\underline{\mathbf{A}}'_{2,4}$ and $\underline{\mathbf{C}}'_{2,4}$. Here, we assume that matrix $_{565}$ this version as <combined> to denote a selected combination 511 B has the row-major format which is why both tensor 566 of cpar-loop and cpar-gemm> functions. 512 slices are also treated as row-major matrices. Notice that 513 gemm in Algorithm 2 will be called with exact same argu- $_{514}$ ments as displayed in the eighth case in Table 1 where 515 $n'_1 = n_{\pi_1}$, $n'_3 = n_q$ and $w_q = w'_3$. For the sake of simplic-516 ity, we omitted the first three arguments of gemm which are 517 set to CblasRowMajor and CblasNoTrans for A and B. With 518 the help of the reshaping operation, the tree-recursion has 519 been transformed into two loops which iterate over all free 520 indices.

521 Matrix Multiplication with Subtensors. An alternative al-₅₂₂ gorithm is given by combining Algorithm 2 with order- \hat{q} $_{523}$ subtensors that have been discussed in 4.3. With order- \hat{q} 524 subtensors, only the outer modes $\pi_{\hat{q}+1},\dots,\pi_p$ are free for 525 parallel execution while the inner modes $\pi_1, \ldots, \pi_{\hat{q}-1}, q$ are $_{526}$ used for the slice-matrix multiplication. Therefore, both 527 tensors are reshaped twice using $\varphi_{\pi_1,\pi_{\hat{q}-1}}$ and $\varphi_{\pi_{\hat{q}+1},\pi_p}$. 528 Note that in contrast to tensor slices, the first reshaping ₅₂₉ also contains the dimension n_{π_1} . The reshaped tensors are 530 of order 3 where $\underline{\mathbf{A}}'$ has the shape $\mathbf{n}' = (\hat{n}_{\pi_1}, n_q, \hat{n}_{\pi_3})$ with $\hat{n}_{\pi_1}=\prod_{r=1}^{\hat{q}-1}n_{\pi_r}$ and $\hat{n}_{\pi_3}=\prod_{r=\hat{q}+1}^pn_{\pi_r}$. Tensor $\underline{\mathbf{C}}'$ has 532 the same dimensions as $\underline{\mathbf{A}}'$ except for $m_2=m$.

Algorithm 2 needs a minor modification for support- $_{534}$ ing order- \hat{q} subtensors. Instead of two loops, the modified 535 algorithm consists of a single loop which iterates over di- $_{\rm 536}$ mension $\hat{n}_{\pi_{\rm 3}}$ calling a single-threaded gemm with subtensors $_{537}$ \mathbf{A}' and \mathbf{C}' . The shape and strides of both subtensors as 538 well as the function arguments of gemm have already been $_{539}$ provided by the previous subsection 4.3. This ttm version 540 will referred to as <par-loop><subtensor>.

Note that functions <par-gemm> and <par-loop> imple-542 ment opposing versions of the ttm where either gemm or the 543 fused loop is performed in parallel. Version <par-loop-gemm 544 executes available loops in parallel where each loop thread $_{545}$ executes a multi-threaded gemm with either subtensors or 546 tensor slices.

547 4.4.3. Combined Matrix Multiplication

The combined matrix multiplication calls one of the 549 previously discussed functions depending on the number 550 of available cores. The heuristic assumes that function 551 cpar-gemm> is not able to efficiently utilize the processor 552 cores if subtensors or tensor slices are too small. The 553 corresponding algorithm switches between <par-loop> and 554 <par-gemm> with subtensors by first calculating the par-555 allel and combined loop count $\hat{n} = \prod_{r=1}^{\hat{q}-1} n_{\pi_r}$ and $\hat{n}' =$ $\prod_{r=1}^{p} n_{\pi_r}/n_q$, respectively. Given the number of physical 557 processor cores as ncores, the algorithm executes <par-loop> 610 libiomp5 has been used for the three BLAS functions gemv, 558 with <subtensor> if ncores is greater than or equal to \hat{n} 559 and call <par-loop> with <slice> if ncores is greater than $_{560}$ or equal to \hat{n}' . Otherwise, the algorithm will default to 561 <par-gemm> with <subtensor>. Function par-gemm with ten-562 sor slices is not used here. The presented strategy is differ-563 ent to the one presented in [14] that maximizes the number

509 the inner one loops over $n_2'=\hat{n}_{\pi_2}$ calling gemm with ten- 564 of modes involved in the matrix multiply. We will refer to

567 4.4.4. Multithreaded Batched Matrix Multiplication

The multithreaded batched matrix multiplication ver-569 sion calls in the eighth case a single gemm batch function 570 that is provided by Intel MKL's BLAS-like extension. With 571 an interface that is similar to the one of cblas_gemm, func-572 tion gemm batch performs a series of matrix-matrix op-573 erations with general matrices. All parameters except 574 CBLAS_LAYOUT requires an array as an argument which is 575 why different subtensors of the same corresponding ten-576 sors are passed to gemm_batch. The subtensor dimensions 577 and remaining gemm arguments are replicated within the 578 corresponding arrays. Note that the MKL is responsible 579 of how subtensor-matrix multiplications are executed and 580 whether subtensors are further divided into smaller sub-581 tensors or tensor slices. This algorithm will be referred to 582 as <batched-gemm>.

583 5. Experimental Setup

584 5.1. Computing System

The runtime benchmark have been executed on a dual 586 socket Intel Xeon Gold 5318Y CPU with an Ice Lake ar-587 chitecture and a dual socket AMD EPYC 9354 CPU with 588 a Zen4 architecture. With two NUMA domains, the Intel 589 CPU consists of 2×24 cores which run at a base frequency 590 of 2.1 GHz. Assuming a peak AVX-512 Turbo frequency 591 of 2.5 GHz, the CPU is able to process 3.84 TFLOPS 592 in double precision. We have measured a peak double-593 precision floating-point performance of 3.8043 TFLOPS 594 (79.25 GFLOPS/core) and a peak memory throughput 595 of 288.68 GB/s using the Likwid performance tool. The 596 AMD EPYC 9354 CPU consists of 2 × 32 cores running at 597 a base frequency of 3.25 GHz. Assuming an all-core boost 598 frequency of 3.75 GHz, the CPU is theoretically capable 599 of performing 3.84 TFLOPS in double precision. We mea-600 sured a peak double-precision floating-point performance 601 of 3.87 TFLOPS (60.5 GFLOPS/core) and a peak memory 602 throughput of 788.71 GB/s.

All libraries have been compiled with the GNU com-604 piler v11.2.0 using the highest optimization level -03 to-605 gether with the -fopenmp and -std=c++17 flags. Loops 606 within the eighth case have been parallelized using GCC's 607 OpenMP v4.5 implementation. In case of the Intel CPU, 608 the Intel Math Kernel Library 2022 (MKL) and its thread-609 ing library mkl_intel_thread, threading runtime library 611 gemm and gemm_batch. For the AMD CPU, the AMD library 612 AOCL v4.2.0 has been used. It has been compiled with 613 the zen4 architecture configuration option and OpenMP 614 threading.

Dataset	Tensor Shape Ex.	Matrix Shape Ex.
N_1	$65536 \times 1024 \times 2$	65536×1024
	$2048 \times 1024 \times 2 \times 2 \times 2$	2048×1024
N_2	$1024 \times 65536 \times 2$	65536×1024
	$1024 \times 2048 \times 2 \times 2 \times 2$	2048×1024
N_3	$1024 \times 2 \times 65536$	65536×1024
	$1024 \times 2 \times 2048 \times 2 \times 2$	2048×1024
N_{10}	$1024 \times 2 \times 65536$	65536×1024
	$1024 \times 2 \times 2 \times 2 \times 2048$	2048×1024
M	$256 \times 256 \times 256$	256×256
	$32\times32\times32\times32\times32$	32×32

Dataset Q (orig. Name)	Tensor Shape	Matrix Shape Ex.
CESM ATM	$26 \times 1800 \times 3600$	1800×26
ISABEL	$100 \times 500 \times 500 \times 13$	500×100
NYX	$512 \times 512 \times 512 \times 6$	512×512
SCALE-LETK	$98 \times 1200 \times 1200 \times 13$	1200×98
QMCPACK	$69 \times 69 \times 115 \times 288$	69×69
Miranda	$256 \times 384 \times 384 \times 7$	384×256
SP	$500 \times 500 \times 500 \times 11$	500×500
EXAFEL	$986 \times 32 \times 185 \times 388$	32×986

Table 2: Tensor shape sets and example dimension tuples that are used in our runtime benchmarking. The first 4 shape sets N₁, N₂, N₃ and N_{10} are used to generate asymmetrically shaped tensors, each consisting of 72 dimension tuples. Shape set M contains 48 tensor shapes that are used to generate symmetrically shaped tensors. Shape set Q contains 8 tensor shapes that are part of SDRBench [24]. Note that all matrix shapes depend on the input tensor shapes and contraction mode.

5.2. OpenMP Parallelization

The loops in the par-loop algorithms have been par-617 allelized using the OpenMP directive omp parallel for to-618 gether with the schedule(static), num_threads(ncores) and 658 5.3. Data sets 619 proc_bind(spread) clauses. In case of tensor-slices, the 620 collapse(2) clause has been added for transforming both 621 loops into one loop which has an iteration space of the 661 account for a wide range of use cases. Their corresponding 622 first loop times the second one. We also had to enable 623 nested parallelism using omp_set_nested to toggle between 624 single- and multi-threaded gemm calls for different TTM 625 cases when using AMD AOCL.

The num_threads(ncores) clause specifies the number 627 of threads within a team where ncores is equal to the 628 number of processor cores. Hence, each OpenMP thread 668 629 is responsible for computing \bar{n}'/ncores independent slice-630 matrix products where $\bar{n}' = n_2' \cdot n_4'$ for tensor slices and $\bar{n}' = n_4'$ for mode- \hat{q} subtensors.

The schedule(static) instructs the OpenMP runtime 633 to divide the iteration space into equally sized chunks, ex-634 cept for the last chunk. Each thread sequentially computes \bar{n}'/ncores slice-matrix products. We have decided 675 or $c \cdot 2^{15-r}$ for $i = \min(r+1,k)$ or 2 otherwise. A special 636 to use this scheduling kind as all slice-matrix multiplica-637 tions exhibit the same number of floating-point operations 677 and the leading dimension are disproportionately large. 638 with a regular workload where one can assume negligible 639 load imbalance. Moreover, we wanted to prevent schedul-640 ing overheads for small slice-matrix products were data 641 locality can be an important factor for achieving higher

The OMP_PLACES environment variable has not been ex-644 plicitly set and thus defaults to the OpenMP cores setting 645 which defines an OpenMP place as a single processor core. 646 Together with the clause num_threads(ncores), the num-647 ber of OpenMP threads is equal to the number of OpenMP 648 places, i.e. to the number of processor cores. We did 688 dimensions $m_{r,c}$ are given by $m_{r,c} = m_{r,1} + (c-1)s_r$ with ₆₄₉ not measure any performance improvements for a higher ₆₈₉ $1 \le c \le 8$. Symmetrically and asymmetrically shaped thread count.

The proc_bind(spread) clause additionally binds each 691 652 OpenMP thread to one OpenMP place which lowers inter- 692 part of the scientific data reduction benchmark (SDR-653 node or inter-socket communication and improves local 693 Bench) [24]. The scientific datasets in SDRBench mainly 654 memory access. Moreover, with the spread thread affin- 694 consist of order-3 tensors with different tensor shapes and

656 OpenMP places which can be beneficial if the user decides 657 to set ncores smaller than the number of processor cores.

We have evaluated the performance of our algorithms 660 with asymmetrically and symmetrically shaped tensors to tensor shapes are divided into 12 sets $N_1, N_2, \ldots, N_{10}, M$ $_{663}$ and Q. Table 2 contains example dimension tuples for the 664 input tensor and matrix. The shape of the latter is (n_2, n_q) 665 if q=1 and (n_1,n_q) otherwise where q is the contraction 666 mode with $1 \leq q \leq p$. The computation of the output 667 tensor dimensions is described in Section 3.2.

The first shape 10 sets N_1 to N_{10} contain 9×8 tensor 669 shapes all of which generate asymmetrically shaped ten-670 sors. Within one set N_k , dimension tuples are arranged ₆₇₁ within 10 two-dimensional shape arrays \mathbf{N}_k of size 9×8 of with $1 \leq k \leq 10$. A dimension tuple $\mathbf{n}_{r,c}$ within \mathbf{N}_k is ₆₇₃ of length r+1 with $1 \le r \le 9$ and $1 \le c \le 8$. Its *i*-th ₆₇₄ element is either 1024 for $i = 1 \land k \neq 1$ or $i = 2 \land k = 1$, 676 feature of this test set is that the contraction dimension

The second shape set M contains 48 tensor shapes that 679 generate symmetrically shaped tensors. The shapes are $_{680}$ arranged within one two-dimensional shape array ${f M}$ of 681 size 6×8 . Similar to the previous setup, the row number $_{682} r$ is equal to the tensor order r+1 with 1 < r6. A row 683 of the tensor shape array consists 8 dimension tuples of 684 the same length r+1 where elements of one dimension 685 tuple are equal such that $m_{r,c} = \mathbf{m}_{r,c}(i) = \mathbf{m}_{r,c}(j)$ for 686 $1 \le i, j \le r+1$. With eight shapes and the step size of 687 each row $s_r = (m_{r,8} - m_{r,1})/8$, the respective intermediate 690 tensors have also been used in [16, 23].

We have also benchmarked with eight tensors that are 655 ity policy, consecutive OpenMP threads are spread across 695 number of data fields, originating from various real-world 696 simulations. Tensors from the SP dataset for instance has 749 <slice> on the Intel Xeon Gold 5318Y CPU. Each contour ₆₉₇ been used for benchmarking the truncated Tucker decom-₇₅₀ level within the plots represents a mean GFLOPS/core 698 position in [21] We perform runtime tests with order-4 ten-699 sors that are generated with dimension tuples of the ten-700 sor shape set Q. Their first three dimensions correspond 753 listed in Table 1. The first column of performance values 701 to the respective ones mentioned in the original data sets 754 is generated by gemm belonging to the TTM case 3, except 702 and the last dimension to the number of data fields. All 703 tensor shapes are provided in Table 2.

704 5.4. Profiling setup

Our benchmark suite iterates through one of tensor 706 shape sets for one contraction mode q with $1 \leq q \leq \max_{p}$ 707 where \max_{p} is the maximum tensor order within the shape 708 set. Tensor and matrix elements are randomly generated 709 single-precision floating-point numbers in case of the data $_{710}$ set Q. In all other cases double-precision is used. The pro-711 filer first sweeps through tensor shapes belonging to one 712 tensor order and then iteratively selects one larger tensor 713 order for the next sweep. It should be noted that if q > p, 714 the contraction mode q is set to p. Given a dimension 715 tuple of length, the profiler generates two tensors and a 716 matrix, executes a mode-q TTM implementation 20 times 717 and finally computes the median runtime of the bench-718 marked TTM implementation. To prevent caching of the 719 output tensor, we invalidate caches which is excluded from 720 the timing.

The runtime results for one contraction mode and one 722 TTM implementation are stored in a two-dimensional ar-723 ray with shape $\max_{p} \times k$ where k is either 8 in case of 724 asymmetrically and symmetrically shaped tensors or 1 in $_{725}$ case of the set Q. Hence, our profiler generates 10 runtime $_{726}$ arrays of shape 9×8 with asymmetrically shaped tensors 727 for 10 contraction modes using the shape sets N_1, N_2, \ldots N_{10} . Generating symmetrically shaped tensors with the $_{729}$ shape set M, the profiler returns 7 runtime arrays of shape $_{730}$ 6 \times 8 for 7 contraction modes. Using the shape set Q, 4 731 one-dimensional runtime arrays for 4 contraction modes 732 are computed.

The three-dimensional runtime data generated with $_{734}$ the data sets N and M can be used to create two dimen-735 sional performance maps, as it is done in the following sec-736 tion 6. Each value in a performance map corresponds to 737 a mean or median value over tensor sizes (i.e. dimension 738 tuples with the same length), over tensor orders or con-739 traction modes. The accumulated mode can be selected 740 depending on the runtime variance.

741 6. Results and Discussion

742 6.1. Slicing Methods

This section analyzes the performance of the two pro-744 posed slicing methods <slice> and <subtensor> that have 745 been discussed in section 4.4. Fig. 1 contains eight per-746 formance contour plots of four ttm functions <par-loop> 747 and <par-gemm>. Both functions either compute the slice-748 matrix product with subtensors <subtensor> or tensor slices

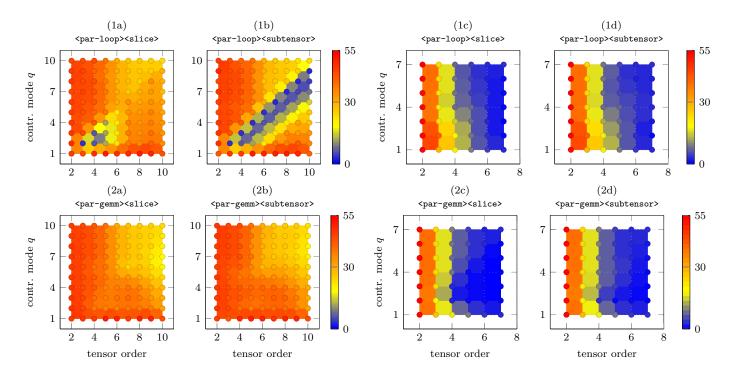
751 value that is averaged across tensor sizes.

Every contour plot contains all applicable TTM cases 755 the first element which corresponds to TTM case 2. The 756 first row, excluding the first element, is generated by TTM 757 case 6 function. TTM case 7 is covered by the diagonal 758 line of performance values when q = p. Although Fig. 759 l suggests that q>p is possible, our profiling program 760 ensures that q=p. TTM case 8 with multiple gemm calls 761 is represented by the triangular region which is defined by

Function <par-loop, slice > runs on average with 34.96 764 GFLOPS/core (1.67 TFLOPS) with asymmetrically shaped 765 tensors. With a maximum performance of 57.805 GFLOP-766 S/core (2.77 TFLOPS), it performs on average 89.64% 767 faster than <par-loop, subtensor>. The slowdown with 768 subtensors at q = p-1 or q = p-2 can be explained by the 769 small loop count of the function that are 2 and 4, respec-770 tively. While function <par-loop, slice> is affected by the 771 tensor shapes for dimensions p=3 and p=4 as well, its 772 performance improves with increasing order due to the in-773 creasing loop count. Function <par-loop, slice> achieves 774 on average 17.34 GFLOPS/core (832.42 GFLOPS) if sym- $_{775}$ metrically shaped tensors are used. If subtensors are used, 776 function <par-loop, subtensor> achieves a mean through-777 put of 17.62 GFLOPS/core (846.16 GFLOPS) and is on 779 formances of both functions are monotonically decreasing 780 with increasing tensor order, see plots (1.c) and (1.d) in 781 Fig. 1.

Function <par-gemm, slice > averages 36.42 GFLOPS/-783 core (1.74 TFLOPS) and achieves up to 57.91 GFLOPS/-784 core (2.77 TFLOPS) with asymmetrically shaped tensors. 786 almost identical performance characteristics and is on av- $_{787}$ erage 3.42% slower than its counterpart with tensor slices. 788 For symmetrically shaped tensors, <par-gemm> with sub-789 tensors and tensor slices achieve a mean throughput 15.98 790 GFLOPS/core (767.31 GFLOPS) and 15.43 GFLOPS/-791 core (740.67 GFLOPS), respectively. However, function 792 <par-gemm, subtensor is on average 87.74% faster than 793 <par-gemm, slice> which is hardly visible due to small per-794 formance values around 5 GFLOPS/core or less whenever q < p and the dimensions are smaller than 256. The 796 speedup of the <subtensor> version can be explained by the 797 smaller loop count and slice-matrix multiplications with 798 larger tensor slices.

Our findings indicate that, regardless of the paralleliza-800 tion method employed, subtensors are most effective with 801 symmetrically shaped tensors, whereas tensor slices are 802 preferable with asymmetrically shaped tensors when both 803 the contraction mode and leading dimension are large.



varying tensor orders p and contraction modes q. The top row of maps (1x) depict measurements of the <par-loop> versions while the bottom row of maps with number (2x) contain measurements of the cpar-gemm> versions. Tensors are asymmetrically shaped on the left four maps (a,b) and symmetrically shaped on the right four maps (c,d). Tensor A and C have the first-order while matrix B has the row-major ordering. All functions have been measured on an Intel Xeon Gold 5318Y.

6.2. Parallelization Methods

831

This subsection compares the performance results of the two parallelization methods, <par-gemm> and <par-loop>, 834 <par-gemm> outperform <par-loop> with any type of slicing. as introduced in Section 4.4 and illustrated in Fig. 1.

With asymmetrically shaped tensors, both cpar-gemm> 808 809 functions with subtensors and tensor slices compute the tensor-matrix product on average with ca. 36 GFLOP-811 S/core and outperform function <par-loop, subtensor> on 812 average by a factor of 2.31. The speedup can be explained 813 by the performance drop of function <par-loop, subtensor> ₈₁₄ to 3.49 GFLOPS/core at q = p - 1 while both versions of <par-gemm> operate around 39 GFLOPS/core. Function <par-loop,slice> performs better for reasons explained in 817 the previous subsection. However, it is on average 30.57% 818 slower than function <par-gemm, slice> due to the aforementioned performance drops.

In case of symmetrically shaped tensors, <par-loop> 821 with subtensors and tensor slices outperform their corre-822 sponding <par-gemm> counterparts by 23.3% and 32.9%, 823 respectively. The speedup mostly occurs when 1 < q < pwhere the performance gain is a factor of 2.23. This performance behavior can be expected as the tensor slice sizes decreases for the eighth case with increasing tensor order 827 causing the parallel slice-matrix multiplication to perform 828 on smaller matrices. In contrast, <par-loop> can execute 829 small single-threaded slice-matrix multiplications in par-830

In summary, function par-loop, subtensor> with sym-

832 metrically shaped tensors performs best. If the leading and 833 contraction dimensions are large, both versions of function

835 6.3. Loops Over Gemm

The contour plots in Fig. 1 contain performance data 837 that are generated by all applicable TTM cases of each 838 ttm function. Yet, the presented slicing or parallelization 839 methods only affect the eighth case, while all other TTM 840 cases apply a single multi-threaded gemm with the same 841 configuration. The following analysis will consider perfor-842 mance values of the eighth case in order to have a more 843 fine grained visualization and discussion of the loops over 844 gemm implementations. Fig. 2 contains cumulative perfor-845 mance distributions of all the proposed algorithms includ-846 ing the functions <batched-gemm> and <combined> for the 847 eighth TTM case only. Moreover, the experiments have 848 been additionally executed on the AMD EPYC processor 849 and with the column-major ordering of the input matrix 850 as well.

The probability x of a point (x,y) of a distribution 852 function for a given algorithm corresponds to the number 853 of test instances for which that algorithm that achieves 854 a throughput of either y or less. For instance, function 855 <batched-gemm> computes the tensor-matrix product with 856 asymmetrically shaped tensors in 25% of the tensor in-857 stances with equal to or less than 10 GFLOPS/core. Please 858 note that the four plots on the right, plots (c) and (d), have 859 a logarithmic y-axis for a better visualization.

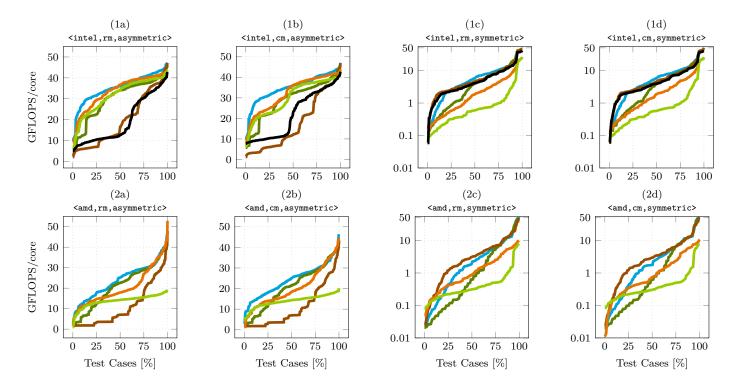


Figure 2: Cumulative performance distributions in double-precision GFLOPS/core of the proposed algorithms for the eighth case. Each distribution belongs to one algorithm: <batched-gemm> (-), <combined> (----), <par-gemm, slice> (---and <par-loop,slice> (<par-gemm.subtensor> () and <par-loop, subtensor> (). The top row of maps (1x) depict measurements performed on an Intel Xeon Gold 5318Y with the MKL while the bottom row of maps with number (2x) contain measurements performed on an AMD EPYC 9354 with the AOCL. Tensors are asymmetrically shaped in (a) and (b) and symmetrically shaped in (c) and (d). Input matrix has the row-major ordering (rm) in (a) and (c) and column-major ordering (cm) in (b) and (d).

6.3.1. Combined Algorithm and Batched GEMM

This subsection discusses the performance of function <batched-gemm> and <combined> against those of <par-loop> and <par-gemm> for the eighth TTM case.

Given a row-major matrix ordering, the combined func-865 tion <combined> achieves on the Intel processor a median 892 contraction modes and leading dimensions. 866 throughput of 36.15 and 4.28 GFLOPS/core with asym-867 metrically and symmetrically shaped tensors. Reaching 893 6.3.2. Matrix Formats 868 up to 46.96 and 45.68 GFLOPS/core, it is on par with 894 869 <par-gemm, subtensor> and <par-loop, slice> and outper-870 forms them for some tensor instances. Note that both 871 functions run significantly slower either with asymmetri-872 cally or symmetrically shaped tensors. The observable su-873 perior performance distribution of <combined> can be at-874 tributed to the heuristic which switches between
900 major and column-major performance values is around 5

100 major and column-major performance values is around 5

100 major and column-major performance values is around 5

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100 major and column-major and column-ma 875 and <par-gemm> depending on the inner and outer loop count as explained in section 4.4.

Function <batched-gemm> of the BLAS-like extension library has a performance distribution that is akin to the <par-loop,subtensor>. In case of asymmetrically shaped 880 tensors, all functions except <par-loop, subtensor> outperform <batched-gemm> on average by a factor of 2.57 and up 882 to a factor 4 for $2 \le q \le 5$ with $q+2 \le p \le q+5$. In 907 6.3.3. BLAS Libraries 883 contrast, <par-loop, subtensor> and <batched-gemm> show 908 884 a similar performance behavior in the plot (1c) and (1d) 909 that use Intel's Math Kernel Library (MKL) on the Intel 885 for symmetrically shaped tensors, running on average 3.55 910 Xeon Gold 5318Y processor with those that use the AMD 886 and 8.38 times faster than set with subtensors and on Optimizing CPU Libraries (AOCL) on the AMD EPYC

887 tensor slices, respectively.

In summary, <combined> performs as fast as, or faster 889 than, <par-gemm, subtensor> and <par-loop, slice>, depend-890 ing on the tensor shape. Conversely, <batched-gemm> un-891 derperforms for asymmetrically shaped tensors with large

This subsection discusses if the input matrix storage 895 formats have any affect on the runtime performance of 896 the proposed functions. The cumulative performance dis-897 tributions in Fig. 2 suggest that the storage format of 898 the input matrix has only a minor impact on the perfor-899 mance. The Euclidean distance between normalized row-901 or less with a maximum dissimilarity of 11.61 or 16.97, in-902 dicating a moderate similarity between the corresponding 903 row-major and column-major data sets. Moreover, their 904 respective median values with their first and third quar-905 tiles differ by less than 5% with three exceptions where the 906 difference of the median values is between 10% and 15%.

This subsection compares the performance of functions

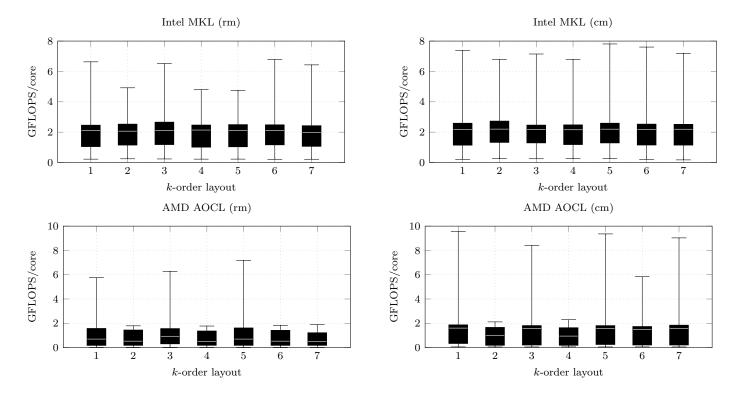


Figure 3: Box plots visualizing performance statics in double-precision GFLOPS/core of the function with row-major (left) or column-major matrices (right). Box plot number k denotes the k-order tensor layout of symmetrically shaped tensors with order 7.

912 9354 processor. Comparing the performance per core and 940 ing <combined> with AOCL, the RSD of its median per-913 limiting the runtime evaluation to the eighth case, MKL- 941 formances for the row-major and column-major formats 914 based functions with asymmetrically shaped tensors run 942 are 25.62% and 20.66%, respectively. The RSD of its re-915 on average between 1.48 and 2.43 times faster than those 943 spective IQRs are 10.83% and 4.31%, indicating a similar 916 with the AOCL. For symmetrically shaped tensors, MKL- 944 performance distributions. A similar performance behav-917 based functions are between 1.93 and 5.21 times faster 945 ior can be observed also for other ttm variants such as 918 than those with the AOCL. In general, MKL-based func-919 tions on the respective CPU achieve a speedup of at least 920 1.76 and 1.71 compared to their AOCL-based counterpart 921 when asymmetrically and symmetrically shaped tensors 922 are used.

6.4. Layout-Oblivious Algorithms

Fig. 3 contains four box plots summarizing the perfor- 952 925 mance distribution of the <combined> function using the AOCL and MKL. Every k-th box plot has been computed from benchmark data with symmetrically shaped order-7 tensors that has a k-order tensor layout. The 1-order and 7-order layout, for instance, are the first-order and last-930 order storage formats of an order-7 tensor.

The reduced performance of around 1 and 2 GFLOPS 932 can be attributed to the fact that contraction and lead-933 ing dimensions of symmetrically shaped subtensors are at 934 most 48 and 8, respectively. When <combined> is used 935 with MKL, the relative standard deviations (RSD) of its 936 median performances are 2.51% and 0.74%, with respect 937 to the row-major and column-major formats. The RSD 938 of its respective interquartile ranges (IQR) are 4.29% and 966 local and distributed TTM function [21]. The local ver-939 6.9%, indicating a similar performance distributions. Us-

946 <par-loop, slice>. The runtime results demonstrate that 947 the function performances stay within an acceptable range 948 independent for different k-order tensor layouts and show 949 that our proposed algorithms are not designed for a spe-950 cific tensor layout.

951 6.5. Other Approaches

This subsection compares our best performing algo-953 rithm with libraries that do not use the LoG approach. 954 TCL implements the TTGT approach with a high-perform 955 tensor-transpose library **HPTT** which is discussed in [11]. $_{956}$ TCL has been used with the same BLAS libraries as TLIB 957 to ensure a fair comparison. TBLIS (v1.2.0) implements 958 the GETT approach that is akin to BLIS' algorithm de-959 sign for the matrix multiplication [12]. The library has 960 been compiled with the zen4 and skx-2 to enable architec-961 ture specific optimization. The tensor extension of Eigen 962 (v3.4.90) is used by the Tensorflow framework. Library 963 LibTorch (v2.5.0) is the C++ distribution of PyTorch 964 [20]. The **TuckerMPI** library is a parallel C++ software 965 package for large-scale data compression which provides a 967 sion implements the LoG approach using a BLAS imple-

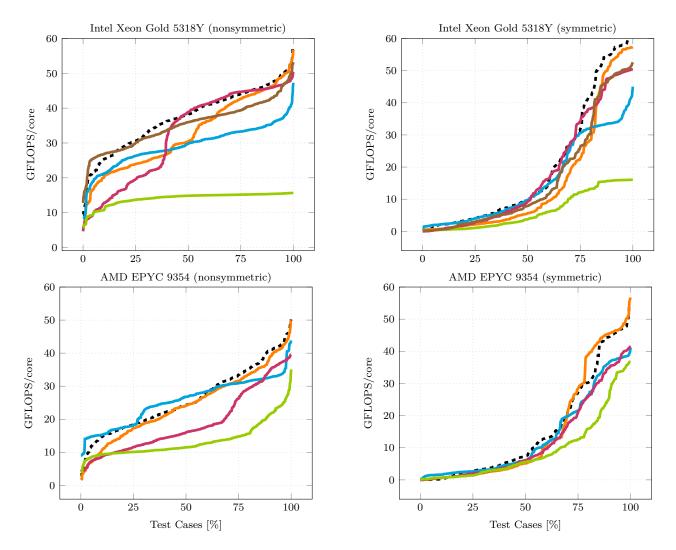


Figure 4: Cumulative performance distributions of TTM implementations in double-precision GFLOPS/core. Each distribution corresponds to a library: TLIB[ours] (---), TCL (--__), TBLIS (____), LibTorch (____ -), Eigen (•), TuckerMPI (= tested with asymmetrically-shaped (left plot) and symmetrically-shaped tensors (right plot).

971 MKL, which is why TuckerMPI's TTM has only been ex-990 pute the TTM with 9.84 and 7.91 GFLOPS/core which is ecuted on the Intel CPU. TLIB denotes our library and 991 only 1.38% and 6.23% slower than TLIB, respectively. the previously discussed <combined> algorithm.

975 implementation with the previously mentioned libraries. 994 reaching a maximum performance of 50.18 GFLOPS/core 976 Using MKL on the Intel CPU, TLIB achieves a median 995 (3.21 TFLOPS) with asymmetrically shaped tensors. TB-977 performance of 38.21 GFLOPS/core (1.83 TFLOPS) and 996 LIS reaches 26.81 GFLOPS/core (1.71 TFLOPS) and is 978 reaches a maximum performance of 57.68 GFLOPS/core 997 slightly faster than TLIB. However, TLIB's upper perfor-979 (2.76 TFLOPS) with asymmetrically shaped tensors from 998 mance quartile with 30.82 GFLOPS/core is slightly larger. 980 the shape set N. TLIB is many tensor instances faster 999 TLIB outperforms the remaining libraries by at least 58.80%. than other libraries and therefore achieves a speedup of 1000 In case of symmetrically shaped tensors, TLIB has a me-982 at least 6.36%. LibTorch and TuckerMPI have almost the 1001 dian performance of 7.52 GFLOPS/core (481.39 GFLOPS). 983 same median performance of 38.17 and 35.98 GFLOPS/- 1002 It outperforms all other libraries by at least 15.38%. We 984 core, yet only reach a peak performance 50.48 and 53.21 1003 have observed that TCL and LibTorch have a median per-985 GFLOPS/core and are 17.47% and 6.97% slower than TLIB. 1004 formance of less than 2 GFLOPS/core in the 3rd and 8th

₉₆₈ mentation and computes the TTM product similar to our ₉₈₇ performance is 8.99 GFLOPS/core (431.52 GFLOPS). Ex-to link the current version of TuckerMPI only with Intel 989 libraries by at least 87.52%. TBLIS and TuckerMPI com-

On the AMD CPU, our implementation with AOCL Fig. 2 compares the performance distribution of our 993 computes TTM with 24.28 GFLOPS/core (1.55 TFLOPS), 986 In case of symmetrically shaped tensors, TLIB's median 1005 TTM case which is less than 6% and 10% of TLIB's me-

Library	Perform	nance [GFL	Speedup $[\%]$		
	Min	Median	Max	Median	
TLIB	9.45	38.27	57.87	-	
TCL	7.14	30.46	56.81	6.36	
TBLIS	8.33	29.85	47.28	23.96	
LibTorch	4.65	38.17	50.48	17.47	
Eigen	5.85	14.89	15.67	170.77	
TuckerMPI	12.79	35.98	53.21	6.97	
TLIB	0.14	8.99	58.14	-	
TCL	0.36	5.64	57.35	3.08	
TBLIS	1.11	9.73	45.03	1.38	
LibTorch	0.02	9.31	50.44	12.98	
Eigen	0.21	3.80	16.06	216.69	
TuckerMPI	0.12	7.91	52.57	6.23	

Library	Perfor	mance [GFI	Speedup $[\%]$		
	Min	Median	Max	Median	
TLIB	2.71	24.28	50.18	-	
TCL	1.67	24.11	49.85	0.57	
TBLIS	9.06	26.81	47.83	0.43	
LibTorch	0.63	16.04	50.84	29.68	
Eigen	4.06	11.49	35.08	117.48	
TLIB	0.02	7.75	54.16	-	
TCL	0.01	5.14	56.75	6.10	
TBLIS	0.06	6.14	41.11	13.64	
LibTorch	0.06	6.04	41.65	12.37	
Eigen	0.07	5.58	36.76	114.22	

Table 3: The table presents the minimum, median, and maximum runtime performances in GFLOPS/core alongside the median speedup of TLIB compared to other libraries. The tests were conducted on an Intel Xeon Gold 5318Y CPU (left) and an AMD EPYC 9354 CPU (right). The performance values on the upper and lower rows of one table were evaluated using asymmetrically and symmetrically shaped tensors,

1006 dian performance with asymmetrically and symmetrically 1044 compute the TTM for the EXAFEL data set which is why 1007 shaped tensors, respectively.

In most instances, TLIB is able to outperform the com- 1046 1009 peting libraries across all TTM cases. However, there 1047 cases faster than other libraries and outperforms them 1010 are few exceptions. On the AMD CPU, TBLIS is about 1048 by at most 137.32% (TCL), 100.80% (TBLIS), 210.71% 1011 12.63% faster than TLIB for the 8th TTM case with asym- 1049 (LibTorch), 798.91% (Eigen), 581.73% (TuckerMPI). TCL 1012 metrically shaped tensors. LibTorch performs in the 7th 1050 is on par with TLIB for the CESM-ATM data set. Tuck-1013 TTM case 1.44% faster than TLIB with asymmetrically 1051 erMPI is 46.8% (CESM-ATM) and 13.7% (Miranda) faster 1014 shaped tensors. One unexpected finding is that LibTorch 1052 than TLIB. More precisely, the TTMs of TuckerMPI and 1015 achieves 96% of TLIB's performance with asymmetrically 1053 LibTorch over the fourth mode is faster than TLIB's TTM 1016 shaped tensors and only 28% in case of symmetrically 1054 for almost all tensor instances. 1017 shaped tensors. On the Intel CPU, LibTorch is on av- 1055 1018 erage 12.64% faster than TLIB in the 7th TTM case. The 1056 than most other libraries except for TCL and LibTorch in 1019 TCL library runs on average as fast as TLIB in the 6th 1057 some instances. TLIB is at most 33.36% (TCL), 117.22% 1020 and 7th TTM cases. The performances of TLIB and TB- 1058 (TBLIS), 221.25% (LibTorch), 205.80% (Eigen) faster. TCL 1021 LIS are in the 8th TTM case almost on par, TLIB run- 1059 outerperforms TLIB by 16.22% (NYX) and 71.65% (Mi-1022 ning about 7.86% faster. In case of symmetrically shaped 1060 randa). In this case, TCL's TTM over the fourth mode 1023 tensors, all libraries except Eigen outperform TLIB by 1061 outperforms TLIB's TTM for almost all tensor instances 1024 about 4.34% (TCL), 38.5% (TBLIS), 67.39% (LibTorch) 1062 and is in case of the SCALE-LETKF data set 3.4x faster. formance in the 8th TTM case, while other libraries only 1065 when computing the tensor product over mode one. reach at most 39.29% of TLIB's median performance.

1030 an order-3 and seven order-4 tensors that have also been 1068 than other libraries for most tensor shapes. 1031 used in SDRBench [24]. The corresponding tensor shape 1032 set Q and the tensor shapes are given in Table 2. With a 1069 6.6. Summary $_{1033}$ maximum tensor order of 4, every tensor is multiplied with $_{1070}$ ¹⁰³⁴ a matrix along every mode using a TTM implementation. ¹⁰⁷¹ function with subtensors and tensor slices. Our findings 1035 Note that the multiplication over the first and fourth mode 1036 corresponds to the sixth and seventh TTM case in Table 1037 1. TLIB will call a single gemm for both cases. The mul-1038 tiplication over the second and third mode corresponds to 1039 the eighth TTM case. Fig. 5 contains bar plots for all $_{1040}$ tensor shapes of set Q. The size of each bar is the total 1041 running time of the respective TTM implementation that $_{1042}$ is executed on an Intel Xeon Gold 5318Y CPU and an 1043 AMD EPYC 9354 CPU. Note that TCL was not able to

1045 the runtime is set to zero.

On the Intel Xeon Gold 5318Y CPU, TLIB is in most

On the AMD EPYC 9354 CPU, TLIB performs better and 4.29% (TuckerMPI) in the 7th TTM case. TBLIS 1063 LibTorch outperforms TLIB for the CESM-ATM data set and TuckerMPI reach 91.78% and 96.87% of TLIB'S per- 1064 by 42.02%. In that case, LibTorch is outperforming 67%

The runtime tests with tensors from the SDRBench 1066 We have additionally conducted performance tests with 1067 illustrates that TLIB is able to compute the TTM faster

We have evaluated the impact of performing the gemm 1072 indicate that, subtensors are most effective with symmet-1073 rically shaped tensors independent of the parallelization 1074 method. Tensor slices are preferable with asymmetrically 1075 shaped tensors when both the contraction mode and lead-1076 ing dimension are large. Our runtime results show that 1077 parallel executed single-threaded gemm performs best with 1078 symmetrically shaped tensors. If the leading and contrac-1079 tion dimensions are large, functions with a multi-threaded 1080 gemm outperforms those with a single-threaded gemm for any

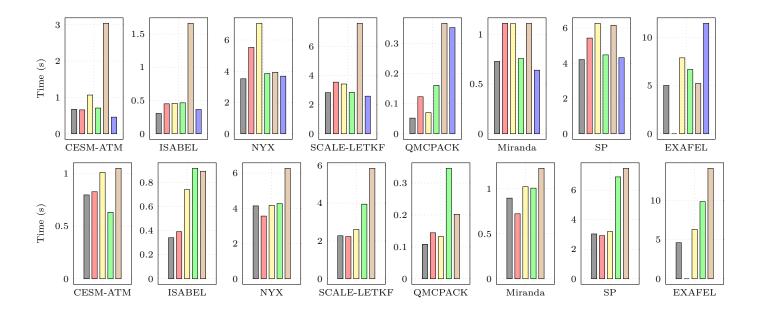


Figure 5: Bar plots contain median runtime in seconds of TLIB (I I I), TCL (I I), TBLIS (I I), LibTorch (I I), Eigen (I II) and TuckerMPI (I II). The tests were conducted on an Intel Xeon Gold 5318Y CPU (top) and an AMD EPYC 9354 CPU (bottom) using order-3 and order-4 tensors with shapes that are described in Table 2.

1081 type of slicing. We have also shown that our <combined> 1111 sors with arbitrary tensor order, dimensions and with any 1082 performs in most cases as fast as <par-gemm, subtensor> and 1112 linear tensor layout all of which can be runtime variable. 1083 <par-loop,slice>, depending on the tensor shape. Func- 1113 1084 tion 1084 tion <a hre 1085 rically shaped tensors with large contraction and leading 1115 cblas_gemm. We have presented multiple algorithm vari-1086 dimensions. While matrix storage formats have only a mi- 1116 ants for the general (eighth) TTM case which either calls 1087 nor impact on TTM performance, runtime measurements 1117 a single- or multi-threaded cblas_gemm with small or large 1088 show that a TTM using MKL on the Intel Xeon Gold 1118 tensor slices in parallel or sequentially. We have applied a 1091 have also demonstrated that our algorithms perform con- 1121 a large set of tensor instances of different shapes, we have 1092 sistently well across different k-order tensor layouts, indi- 1122 evaluated the proposed variants on an Intel Xeon Gold 1093 cating that they are layout-oblivious and do not depend 1123 5318Y and an AMD EPYC 9354 CPUs. 1094 on a specific tensor format. Our runtime tests show that 1095 TLIB'S function <combined> is, in median, between 15.38% and 257.58% faster than other competing libraries, except 1097 for TBLIS. TLIB is either on par with or slightly outper-1098 forms TBLIS for many tensor shapes which uses optimized 1126 layout-oblivious and do not need layout-specific optimiza-1099 kernels for the TTM computation. Table 3 contains the 1127 tions, even for different storage ordering of the input ma- $_{1100}$ minimum, median, and maximum runtime performances $_{1128}$ trix. Despite the flexible design, our best-performing al-1101 including TLIB's speedups for the whole tensor test sets.

7. Summary

 $_{1104}$ for the compute-bound tensor-matrix multiplication that $_{1134}$ most state-of-the-art implementations. 1105 is essential for many tensor methods. Our approach is 1135 1106 based on the LOG-method and computes the tensor-matrix 1136 viable solution for the general tensor-matrix multiplication product in-place without transposing tensors. It applies 1137 which can be as fast as or even outperform efficient GETT-1108 the flexible approach described in [16] and generalizes the 1138 based implementations. Hence, other actively developed 1109 findings on tensor slicing in [14] for linear tensor layouts. 1139 libraries such as LibTorch, TuckerMPI and Eigen might 1110 The resulting algorithms are able to process dense ten- 1140 benefit from implementing the proposed algorithms. Our

The base algorithm has been divided into eight dif-5318Y CPU achieves higher per-core performance than a 1119 simple heuristic that selects one of the variants based on TTM with AOCL on the AMD EPYC 9354 processor. We 1120 the performance evaluation in the original work [1]. With

1124 8. Conclusion and Future Work

Our performance tests show that our algorithms are 1129 gorithm is able to outperform Intel's BLAS-like extension 1130 function cblas_gemm_batch by a factor of 2.57 in case of 1131 asymmetrically shaped tensors. Moreover, the presented 1132 performance results show that TLIB is able to compute We have presented efficient layout-oblivious algorithms 1133 the tensor-matrix product in median 15.38% faster than

> Our findings show that the LoG-based approach is a 1141 header-only library provides C++ interfaces and a python

1142 module which allows frameworks to easily integrate our 1207 [16] C. Bassoy, Design of a high-performance tensor-vector multi-1143 library.

In the near future, we intend to incorporate our im- $_{1145}$ plementations in TensorLy, a widely-used framework for $_{1211}$ 1146 tensor computations [25, 19]. Using the insights provided 1212 1147 in [14] could help to further increase the performance. Ad- 1213 [18] 1148 ditionally, we want to explore to what extend our approach 1149 can be applied for the general tensor contractions.

1150 8.0.1. Source Code Availability

Project description and source code can be found at ht 1152 tps://github.com/bassoy/ttm. The sequential tensor-matrix 1153 multiplication of TLIB is part of Boost's uBLAS library.

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