Communication Lower Bounds of Bilinear Algorithms for Symmetric Tensor Contractions

Edgar Solomonik ∗ James Demmel † Torsten Hoefler ‡

July 18, 2017

Abstract

Accurate numerical calculations of electronic structure are often dominated in cost by tensor contractions. These tensors are typically symmetric under interchange of modes, enabling reduced-size representations as well as a reduced computation cost. Direct evaluation algorithms for such contractions use matrix and vector unfoldings of the tensors, computing and accumulating products of input elements. Symmetry preserving algorithms reduce the number of products by multiplying linear combinations of input elements. The two schemes can be encoded via sparse matrices as bilinear algorithms. We formulate a general notion of expansion for bilinear algorithms in terms of the rank of submatrices of the sparse matrix encoding. This expansion bounds the number of products that can be computed provided a bounded amount of data. Consequently, we derive communication lower bounds for any sequential or parallel schedule of a bilinear algorithm with a given expansion. After deriving such expansion bounds for the tensor contraction algorithms, we obtain new results that demonstrate asymptotic communication overheads associated with exploiting symmetries. Computing a nonsymmetric tensor contraction requires less communication than either method for symmetric contractions when either (1) computing a symmetrized tensor-product of tensors of different orders or (2) the tensor unfolding of the contraction corresponds to a matrix–vector product with a nonsquare matrix. Further, when the unfolding is a product of two non-square matrices, asymptotically more communication is needed by the symmetry preserving algorithm than the traditional algorithm, despite its lower computation cost.

1 Introduction

Tensor contractions are tensor products that are summed (contracted) over a subset of the modes (indices). They generalize the product of a matrix and a vector and of two matrices as well as provide an algebra that is widely used in electronic structure calculations in quantum chemistry. Tensor representations allow expression of different types of electron–orbital interactions as different contractions. Tensors representing multi-electron and multi-orbital interactions encode interchangeability of these entities as permutational symmetries in the data representation [4]. While any contraction may be reduced to a product of two matrices (or vectors), such reductions are suboptimal in computation cost for tensors with symmetry. Algebraic reorganization of the contractions can yield reductions in computation cost ranging from 2X for contractions in common methods such as CCSD to 4X and 9X for contractions in higher-order methods (CCSDT and CCSDTQ respectively) [22]. In this paper, we compare the communication cost of reducing the contractions of symmetric tensors to matrix multiplication (the direct evaluation algorithm) to executing the algebraically reorganized form (the symmetry preserving algorithm).

We formalize the problem of a symmetric contraction, as the contraction of two symmetric tensors and subsequent symmetrization of the result. Symmetrization involves taking the sum of all permutations of the initial contraction product and results in a symmetric tensor. Electronic structure methods employ symmetrization, but additionally also involve antisymmetric tensors, antisymmetrization, as well as partial symmetries. We consider exclusively symmetric tensors [8] (otherwise referred to as fully symmetric or supersymmetric [13]). The relevant algorithms for antisymmetric tensors are similar in structure [22], but extension of our results to partially symmetric tensors is nontrivial.

Our algorithms are defined algebraically by a set of products of linear combinations of inputs and partial summations of these bilinear forms. Each of these algorithms can be encoded by a set of three sparse matrices as a...
bilinear algorithm [17]. We derive the communication requirements of any bilinear algorithm with a provided expansion bound. This expansion bound is an algorithm-specific function relating the ranks of submatrices of the three sparse matrices. Given this infrastructure, it suffices to derive expansion bounds for each bilinear algorithm to obtain communication lower bound results. We leverage the Loomis-Whitney inequality [15, 25] to prove expansion bounds based on the sparsity structure of the matrices encoding each algorithm.

Our bilinear algorithm representation and rank-based communication lower-bounds are more concise, powerful, and extensible than previous models. By working with rank of the matrices encoding bilinear algorithms, we permit schedules to form arbitrary intermediates. Further, nested bilinear algorithms are defined by the tensor products of the matrices representing each algorithm in the nest. This property suggests that our work can be extended to fast matrix multiplication algorithms such as [24], as well as to partially-symmetric contraction algorithms.

To formally obtain communication lower bounds, we also need to carefully characterize the notion of sequential and parallel execution. We associate an execution DAG (directed acyclic graph) with a particular specification of a bilinear algorithm (multiple execution DAGs are possible for a single bilinear algorithm). We then consider potential sequential schedules and parallel schedules of execution DAGs. We measure the vertical communication cost of a sequential schedule as the amount of data moved between memory and a single level of cache. We measure the horizontal communication cost of a parallel schedule as the amount of data communicated between any one processor and the others. Our horizontal communication lower bounds can be translated to the LogGP [1] or BSP [26] models. Our execution model disallows recomputation of any operation defined in the algorithm during the schedule execution. We further assume that each unique tensor element is initially stored on a unique processor and that the number inputs and outputs are load balanced across processors.

Our main results are lower bounds on vertical and horizontal communication costs of any sequential or parallel schedule for the direct evaluation and symmetry preserving algorithms for symmetric tensor contractions. Nonsymmetric tensor contractions may be unfolded into matrix or vector products of the tensors, by uniting the contracted modes and, for both the operands, uniting the rest of the modes, yielding a total of up to three modes (matrix–matrix multiplication). All tensor contractions where none of the three tensors (two input and one output) is a scalar, can be characterized as either matrix-vector-like or matrix-matrix-like based on this unfolding. As we analyze only symmetric contractions, all tensor dimensions are equal, however, the tensor unfoldings may be non-square matrices when different numbers of modes are folded into the two matrix dimensions. Our lower bounds are the same for all algorithms when the three unfolded tensors are either square matrices or vectors. However, when at least one of the three tensor unfoldings is a nonsquare matrix, we obtain the following lower bounds, which are asymptotically higher (i.e. stronger) than known results.

- For matrix-vector-like contractions, the direct evaluation algorithm and symmetry preserving algorithm require less computation, but asymptotically more horizontal communication than a nonsymmetric contraction with the same dimensions,
  - when the unfolding is a vector outer product (the contraction is a symmetrized tensor product), extra communication is necessitated by symmetrization,
  - when the unfolding is a matrix-vector product, extra communication is necessitated by symmetric-packed storage of the tensor operands.

- For matrix-matrix-like contractions, the symmetry preserving algorithm requires fewer products, and often less computation, but asymptotically more vertical and horizontal communication than the direct evaluation algorithm.

Our results are summarized for general symmetric contractions (Definition 2.8) as well as some particular instances, at the end of the paper in Table 10.1.

2 Tensor Notation

We use the notation from the introductory work on the symmetry preserving algorithm [22] with some modifications. We additionally restrict all elements of tensors to be in the same algebraic ring. More general definitions of elements and element-wise operations in contractions enable the extension of the formalism and algorithms to partially symmetric contractions [22], which are beyond the scope of this paper.
Our notation departs from standard notation conventions used in the tensor decomposition literature [13], due to our need to work with variable-order tensors and contractions over arbitrary sets of modes. We leverage the fact that different modes of a symmetric tensor are indistinguishable to keep our notation as concise and descriptive as possible. Some basic conventions we employ include denoting tensors (including vectors and matrices) in bold font and denoting vectors with lower-case letters (variable-order tensors are denoted as upper-case letters even when they can be vectors). However, elements of tensors (and of vectors) are denoted in regular (non-bold) font. To distinguish labels from index notation, for tensors and scalar variables we place the label in parentheses, e.g. $T^{(1)}$, $s^{(A)}$.

**Definition 2.1.** We denote a $d$-tuple of integers using vector notation as $\vec{i} := (i_1, \ldots, i_d)$.

These tuples will be used as tensor indices, and each will most often range from 1 to $n$, so $\vec{i} \in [1, n]^d$. We concatenate tuples using the notation $\vec{i} \vec{j} := (i_1, \ldots, i_d, j_1, \ldots, j_f)$ for any $\vec{j} \in [1, n]^f$. We concatenate intervals accordingly $[1, n]^d [1, n]^f = [1, n]^{d+f}$.

**Definition 2.2.** We refer to the space of increasing $d$-tuples with values between 1 and $n$ as $\lessgtr [1, n]^d \iff \vec{i} : i_1 \leq \ldots \leq i_d, \vec{i} \in [1, n]^d$. We also refer to the space of strictly increasing tuples as $\lessgtr [1, n]^d = \vec{i} : i_1 < \ldots < i_d, \vec{i} \in [1, n]^d$.

The number of increasing $d$-tuples between 1 and $n$ is given by $|\lessgtr [1, n]^d| = \left( \begin{array}{c} n+d-1 \end{array} \right)$. The set of increasing tuples will be useful in our algorithms, as $\lessgtr [1, n]^d$ enumerates the unique tensor entries of an order $d$ symmetric tensor (defined below).

**Definition 2.3.** A tensor $T$ with order $d$ and all dimensions $n$ is a collection (multiset),

$$ T := \left( T_{\vec{i}} : \vec{i} \in [1, n]^d \right). $$

We will usually consider tensors with all dimensions equal to $n$. Given an order $d$ tensor $A$, we will refer to its elements using the notation $A_{\vec{i}} = A_{i_1, \ldots, i_d}$.

**Definition 2.4.** For any $s, t, v \geq 0$ with $\omega := s + t + v$, we denote a tensor contraction over $v$ indices between tensor $A$ of order $s + v$ and tensor $B$ of order $v + t$, into tensor $C$ of order $s + t$ each with all dimensions equal to $n$ as

$$ C = A \otimes_v B := \forall \vec{i} \vec{j} \in [1, n]^{s+t}, \quad C_{\vec{i}\vec{j}} = \sum_{\vec{k} \in [1, n]^v} A_{\vec{k}\vec{j}} \cdot B_{\vec{k}\vec{i}}. \quad (2.1) $$

Throughout further contraction definitions and algorithms we will always denote $\omega := s + t + v$ and assume $n \gg \omega$. We employ the notation $A \otimes_v B$, since when $v = 0$, the operator $\otimes_0$ is equivalent to the tensor product, which is commonly denoted as $\otimes$.

**Definition 2.5.** We refer to contractions with exactly one of $s, t, v$ is zero, as matrix-vector-like and contractions with $s, t, v > 0$ as matrix-matrix-like.

We define symmetric tensors and symmetrized contractions by considering all possible permutations of their indices. For this task, we introduce the following permutation notation.

**Definition 2.6.** Let $\Pi_d$ be the set of all possible $d$-dimensional permutation functions, where each $\pi \in \Pi_d$ is associated with a unique bijection $\hat{\pi} : [1, d] \leftrightarrow [1, d]$, as $\pi(\vec{i}) := (i_{\hat{\pi}(1)}, \ldots, i_{\hat{\pi}(d)})$, so $|\Pi_d| = d!$. We denote the collection of all permutations of a tuple $\vec{i}$ as

$$ \Pi(\vec{i}) := \left( \pi(\vec{i}) : \pi \in \Pi_d \right). $$

**Definition 2.7.** We say an $n$-dimensional order-$d$ tensor $T$ is symmetric if

$$ \forall \vec{i} \in [1, n]^d, \vec{j} \in \Pi(\vec{i}), \quad T_{\vec{i}} = T_{\vec{j}}. $$

According to Definition 2.7, scalars and vectors are symmetric tensors of order 0 and 1, respectively.

**Definition 2.8.** For any $s, t, v \geq 0$, a symmetric contraction is a contraction between symmetric tensors $A$ and $B$ into $C$, where the result is symmetrized, i.e.

$$ C = A \circ_v B := \forall \vec{i} \in [1, n]^{s+t}, \quad C_{\vec{i}} = \sum_{\vec{j} \in \Pi(\vec{i})} \left( \sum_{\vec{k} \in [1, n]^v} A_{\vec{k}\vec{j}} \cdot B_{\vec{k}\vec{i}} \right). \quad (2.2) $$
The resulting tensor $\mathbf{C}$ satisfying (2.2) is always symmetric. For $(s = 1, t = 0, v = 1)$, (2.2) corresponds to the product of a symmetric matrix $\mathbf{A}$ with a vector $\mathbf{b}$, $\mathbf{A} \circ_1 \mathbf{b} := \mathbf{Ab}$. For $(s = 1, t = 1, v = 0)$ and commutative ‘‘,’’ (2.2) becomes the rank-two outer product of a column vector $\mathbf{a}$ and a row vector $\mathbf{b}$, $\mathbf{a} \circ_0 \mathbf{b} := \mathbf{ab} + \mathbf{b}^\top \mathbf{a}^\top$. These two vector routines are members of the BLAS [14] and are building blocks in a multitude of numerical routines. For $(s = 1, t = 1, v = 1)$ and commutative ‘‘,’’ (2.2) becomes symmetrized multiplication of symmetric $n \times n$ matrices $\mathbf{A}$ and $\mathbf{B}$, $\mathbf{C} = \mathbf{A} \circ_1 \mathbf{B} := \mathbf{AB} + \mathbf{BA}$. Our definition of symmetric contractions can be extended to scenarios where the operands and/or the result are partially symmetric via nested tensors [22].

While we will define symmetrization in contractions as summing over all possible permutations of the tensor indices (for any $\vec{i}$ the collection $\Pi(\vec{i})$), our algorithms will exploit the equivalence of many of these permutations. As a result, they will need to sum over a set of partitions rather than a full set of permutations, which we define below.

**Definition 2.9.** We define the disjoint partition $\chi^p_q(\vec{k})$ as the collection of all pairs of tuples of size $p$ and $q$, which are disjoint subcollections of $\vec{k}$ and preserve the ordering of elements in $\vec{k}$. We additionally define $\bar{\chi}^p_q(\vec{k})$ as the set of all unique pairs in $\chi^p_q(\vec{k})$.

In other words, if $k_i$ and $k_j$ appear in the same tuple (partition) and $i < j$, then $k_i$ must appear before $k_j$. For example, the possible ordered partitions of $\vec{k} = (k_1, k_2, k_3)$ into pairs of tuples of size one and two are the collection,

$$\chi^1_2(\vec{k}) = \{(k_1, (k_2, k_3)), (k_2, (k_1, k_3)), (k_3, (k_1, k_2))\}.$$

The collection $\chi^p_q(\vec{k})$ can be constructed inductively [22]. The set $\bar{\chi}^p_q(\vec{k})$ will be used whenever we want to exclude equivalent pairs in $\chi^p_q(\vec{k})$ (these exist only when $\vec{k}$ has repeating entries).

**Definition 2.10.** We denote all possible ordered subcollections of a tuple $\vec{k} \in [1, n]^{d+\ell}$ via projection map $\chi^d$,

$$\chi^d(\vec{k}) := \{\vec{i} : (\vec{i}, \vec{j}) \in \chi^2_1(\vec{k})\}.$$ 

In certain cases, our algorithms compute summations over groups of indices of symmetric tensors by summing only over the unique values and scaling by the following multiplicative factor.

**Definition 2.11.** Let $\rho(\vec{k}) := v! / \prod_{i=1}^{\ell} m_i!$ where $m_i$ is the multiplicity of the $i$th of $1 \leq l \leq v$ unique values in $\vec{k}$.

The factor $\rho(\vec{k})$ is the number of unique permutations of $\vec{k}$, i.e. unique values in the collection $\Pi(\vec{k})$.

### 3 Bilinear Algorithms for Tensor Contractions

Tensor contractions $(\mathbf{A} \otimes \mathbf{v}, \mathbf{B})$ and symmetric tensor contractions $(\mathbf{A} \circ \mathbf{B})$ produce a set of bilinear forms (partial sums of products) of the elements of $\mathbf{A}$ and $\mathbf{B}$. We will define direct algorithms that compute these bilinear forms naively by computing all unique products of input elements and accumulating them to the specified partial sums. These algorithms follow directly from the algebraic definitions of $\mathbf{A} \otimes \mathbf{v}$, $\mathbf{B}$ and $\mathbf{A} \circ \mathbf{B}$ given in Section 2. We then consider algorithms that compute a smaller set of products of linear combinations of input elements and obtains the specified partial sums as linear combinations of these. We then provide specifications of them as bilinear algorithms [17], representing each algorithm as a 3-tuple of sparse matrices.

#### 3.1 Nonsymmetric Contraction Algorithm

Nonsymmetric tensor contractions are reducible to matrix multiplication. So, we first consider the trivial algorithm which contracts nonsymmetric tensors $\mathbf{A}$ and $\mathbf{B}$ by evaluating the products in (2.1), which corresponds to standard matrix multiplication.

**Algorithm 3.1** $(\Upsilon^{(s,t,v)})$. For any tensor contraction $\mathbf{C} = \mathbf{A} \otimes \mathbf{v}$, $\mathbf{B}$ we define $\mathbf{C} = \Upsilon^{(s,t,v)}(\mathbf{A}, \mathbf{B})$ to evaluate the multiplications explicitly described by (2.1) in Definition 2.4.
Algorithm 3.1 is equivalent to a multiplication of a matrix $\bar{A}$ with dimensions $n^s \times n^v$, where each row corresponds to $\bar{j} \in [1, n]^{s}$ and each column corresponds to $\bar{k} \in [1, n]^{v}$, by a matrix $\bar{B}$ with dimensions $n^v \times n^t$, where each row corresponds to $\bar{k} \in [1, n]^{v}$ and each column corresponds to $\bar{i} \in [1, n]^{t}$, yielding a matrix $\bar{C}$ with dimensions $n^s \times n^t$. $\bar{C}$ contains all elements of $C = A \otimes_v B$.

When $s, t, v > 0$, we could alternatively employ a different matrix multiplication algorithm to compute (2.1) (e.g. Strassen’s algorithm [24]). In this paper, we will not consider such fast matrix multiplication algorithms, focusing instead on algorithms that exploit symmetry.

### 3.2 Direct Evaluation Algorithm for Symmetric Contractions

The nonsymmetric algorithm may be used to compute symmetric contractions with the additional step of symmetrization of the result of the multiplication between $A$ and $B$. However, when $A$ and $B$ are symmetric, most of the scalar multiplications (products) in (2.2) are equivalent. The following algorithm evaluates $A \circ_v B$ by computing only the unique multiplications and scaling them appropriately.

In particular, since $C$ is symmetric, it is no longer necessary to compute all possible orderings of the indices $\bar{i} \in [1, n]^{s+t}$ in $A \circ_v B$, but only those in increasing order $\bar{i} \in [1, n]^{s+t}$ as these include all unique values of $C$. Further, permutations of the $\bar{k}$ index group result in equivalent scalar multiplications due to symmetry of $A$ and of $B$. In the following algorithm, we rewrite (2.2) to sum over only the ordered sets of these indices and scale them by an appropriate prefactor.

**Algorithm 3.2 ($\Psi_o^{(s,t,v)}$).** For any symmetric contraction $C = A \circ_v B$ compute

$$
C = \Psi_o^{(s,t,v)}(A, B) := \forall \bar{i} \in [1, n]^{s+t}, C_{\bar{i}} = s!t! \sum_{(\bar{j}, \bar{l}) \in \chi_2(\bar{i})} \left( \sum_{\bar{u} \in [1, n]^v} \rho(\bar{k}) A_{\bar{j}\bar{k}} \cdot B_{\bar{k}\bar{l}} \right),
$$

where $\rho(\bar{k})$ is given in Definition 2.11

The algorithm $\Psi_o^{(s,t,v)}$ is algebraically equivalent to (2.2) and is numerically stable [22].

Modulo the scaling by $s!t!$ and $\rho(\bar{k})$, the inner summation of Algorithm 3.2 is equivalent to a matrix multiplication of a matrix $\bar{A}$ with dimensions $\binom{n}{s} \times \binom{n}{s}$ (where each row corresponds to $\bar{j} \in [1, n]^s$ and each column corresponds to $\bar{k} \in [1, n]^v$) by a matrix $\bar{B}$ with dimensions $\binom{n}{v} \times \binom{n}{v}$ (where each row corresponds to $\bar{k} \in [1, n]^v$ and each column corresponds to $\bar{i} \in [1, n]^t$), yielding a matrix $\bar{C}$ with dimensions $\binom{n}{s} \times \binom{n}{v}$. The matrix $\bar{C}$ can be treated as a partially symmetric tensor of order $s + t$ (symmetric in the permutation within the first $s$ indices and within the last $t$ indices) and can be further symmetrized to obtain $C = A \circ_v B$:

$$
\forall \bar{i} \in [1, n]^{s+t}, C_{\bar{i}} = s!t! \sum_{(\bar{j}, \bar{l}) \in \chi_2(\bar{i})} C_{\bar{j}\bar{l}}.
$$

The scaling by $\rho(\bar{k})$ can be applied to the elements of $\bar{A}$ or of $\bar{B}$.

### 3.3 Symmetry Preserving Tensor Contraction Algorithm

The symmetry preserving tensor contraction algorithm below computes symmetric contractions with fewer multiplications and in some cases fewer total operations than the direct evaluation algorithm [22]. It has a number of applications in both matrix computations and high-order coupled cluster [27] tensor contractions. The algorithm requires the computation of a few intermediate tensors, but for brevity we only give the formula for the highest order intermediate tensor (order $\omega = s + t + v$) computed by the algorithm (the rest may be computed using $O(n^{\omega-1})$ multiplications), which suffices for our lower bound derivations.

In the definition of the algorithm, we employ the symbol $\leftarrow$ to denote accumulation, which implies assignment the first time it is applied to a new element and addition afterward, i.e.

$$
a = \sum_{i=1}^{n} b_i \quad \equiv \quad \forall i \in [1, n], a \leftarrow b_i.
$$

This notation reveals the symmetry of the computation with respect to operations on $A$, $B$, and a tensor $Z$ whose elements have a one-to-one correspondence to those in $C$. 

5
Algorithm 3.3 ($\Phi_0^{(s,t,v)}$). For any symmetric contraction $C = A \circ_v B$, compute
\[
\forall i \in [1, n]^w, \quad j \in \chi^{s+t}(\bar{i}), \quad \hat{A}_{ij} \gets A_{ij}, \tag{3.2}
\]
\[
\bar{i} \in \chi^{s+t}(\bar{i}), \quad \hat{B}_{ij} \gets B_{ij}, \tag{3.3}
\]
\[
\mathbf{Z}_{\bar{i}} = \hat{A}_{\bar{i}} \cdot \hat{B}_{\bar{i}} \tag{3.4}
\]
\[
\mathbf{Z}_{\hat{h}} \in \chi^{s+t}(\bar{i}), \quad \mathbf{Z}_{\hat{h}} \gets \mathbf{Z}_{\bar{i}}. \tag{3.5}
\]

Then compute $C = \text{sort}[(Z - V - W)]$, where formulas for computing $V$ and $W$ are given in [22].

The $Z$ tensor contains all terms needed by $C = A \circ_v B$ as well as some extra terms which are independently computed as tensors $V$ and $W$ then subtracted out from $Z$. The computation of $V$ and $W$ can always be done via a low order number of multiplications, but sometimes requires a constant factor more additions than those needed to compute $Z$. The most basic instance of the symmetry preserving algorithm is symmetric matrix vector multiplication, $c = A \circ_1 b := Ab$, for which the algorithm needs to compute $V$, but not $W$,
\[
\forall i \in [1, n], \quad j \in [i, n], \quad \hat{A}_{ij} = A_{ij}, \quad \hat{B}_{ij} = b_i + b_j, \quad \mathbf{Z}_{ij} = \hat{A}_{ij} \cdot \hat{B}_{ij},
\]
\[
\mathbf{Z}_i = \sum_{k=1}^{i} \mathbf{Z}_{ki} + \sum_{k=i+1}^{n} \mathbf{Z}_{ik}, \quad A_i^{(1)} = \sum_{k=1}^{n} A_{ik}, \quad V_i = A_i^{(1)} \cdot b_i, \quad c_i = Z_i - V_i.
\]
The advantage of $c = A \circ_1 b$ is that it requires only $(1/2)n^2$ multiplications to leading order instead of the usual $n^2$. The tensor $W$ needs to be computed only when $s$ and $t$ are greater than zero, the most basic example of which is the symmetrized vector outer product [22].

The correctness proof, numerical stability proof, numerical tests, computation cost analysis, adaptations from symmetric to partially symmetric, antisymmetric, and Hermitian cases, as well as applications are given in [22]. A special case of the symmetry preserving algorithm has also previously been used to accelerate a costly partially-symmetric contraction in one electronic structure method [16]. The symmetry preserving algorithm has no correspondence to a matrix multiplication unlike $\Psi_0^{(s,t,v)}$ and $\Phi_0^{(s,t,v)}$, which makes its communication cost analysis different and interesting.

### 3.4 Bilinear Algorithms

Bilinear algorithms [17] provide a unified algebraic representation for all algorithms above.

Algorithm 3.4 ($\Lambda^2$). Given input vectors $a$, $b$, a bilinear algorithm, defined by matrices $\mathcal{F} = (F^{(A)}, F^{(B)}, F^{(C)})$ (with values in $\mathbb{R}$), computes output vector $c$ via
\[
c = \Lambda^2(a, b) := F^{(C)}[(F^{(A)}a) \odot (F^{(B)}b)],
\]
where $\odot$ is the Hadamard (pointwise) product. We assume the bilinear algorithm is irreducible, i.e. each of the matrices in $\mathcal{F}$ has full row rank.

For typical bilinear algorithms the three matrices in $\mathcal{F}$ are very sparse. For instance, the classical matrix multiplication algorithm, has only one (unit) entry in each column of the three matrices. The number of rows in $F^{(A)}$, $F^{(B)}$, $F^{(C)}$ is equal to the dimension of $a$, $b$, $c$, respectively. We refer to this 3-tuple of dimensions of $a$, $b$, $c$ as $\dim(\Lambda^2) = (\dim(a), \dim(b), \dim(c))$. There is an equal number of columns in the three matrices $F^{(A)}$, $F^{(B)}$, $F^{(C)}$, the number of which is referred to as the rank of the bilinear algorithm, which we denote by $\text{rank}(\Lambda^2)$. The rank of the bilinear algorithm defines the number of scalar multiplications in the Hadamard product, which corresponds to the number of products the algorithm computes. In other words, each column of the sparse matrices in $F^{(A)}$ and $F^{(B)}$ defines the linear combination of inputs (elements of $a$ or of $b$) that contribute to a particular product. Each row of $F^{(C)}$ defines how each output element of $c$ is computed as a linear combination of products.

We now define a representation for bilinear tensor algorithms. Each bilinear tensor algorithm is reducible to a bilinear algorithm in the above representation. The utility of the tensor representation is to succinctly express algorithms for tensor contractions as bilinear algorithms.
Algorithm 3.5 ($\tilde{\Lambda}^{(s,t,v)}_{(D,K)}$). Given tensors $A$, $B$, the bilinear tensor algorithm computes tensor $C$. The three tensors have domains of unique values given by $D := (D^{(A)}, D^{(B)}, D^{(C)}, D^{(M)})$ where $D^{(A)} \subseteq [1,n]^{s+v}$, $D^{(B)} \subseteq [1,n]^{v+t}$, $D^{(C)} \subseteq [1,n]^{s+t}$, and $D^{(M)} \subseteq [1,n]^ω$ (as before $ω = s + t + v$). The algorithm computes the products specified by $K := (K^{(A)}, K^{(B)}, K^{(C)})$ where $K^{(A)}$, $K^{(B)}$, and $K^{(C)}$ are (sparse) tensors (with values in $R$) of orders $[1,n]^{s+v+ω}$, $[1,n]^{s+t+ω}$, and $[1,n]^{s+t+ω}$, respectively. The bilinear algorithm computes the tensor $C$ by evaluating the following set of products (corresponding to intermediate tensor $T$):

$$\forall \tilde{t} \in D^{(M)}, \quad T_{\tilde{t}} = \left( \sum_{j\in D^{(A)}} K^{(A)}_{ji} A_{j}^{\tilde{t}} \right) \cdot \left( \sum_{l\in D^{(B)}} K^{(B)}_{li} B_{l}^{\tilde{t}} \right),$$

then it accumulates these products to compute $C$,

$$\forall \tilde{h} \in D^{(C)}, \quad C_{\tilde{h}} = \sum_{\tilde{t}\in D^{(M)}} K^{(C)}_{\tilde{h}\tilde{t}} T_{\tilde{t}}.$$  

To obtain a bilinear algorithm $\Lambda^{(F)}$ from $\tilde{\Lambda}^{(s,t,v)}_{(D,K)}$ it suffices to enumerate the domains in $D$, mapping the corresponding four index sets to four indices. So, the bilinear algorithm simply corresponds to ‘unfoldings’ [13] of the tensors, $K$, used in the bilinear tensor algorithm into matrix representations, $F$. Thus, the bilinear algorithm will satisfy $\dim(\Lambda^{(F)}) = (|D^{(A)}|, |D^{(B)}|, |D^{(C)}|)$ and $\rank(\Lambda^{(F)}) = |D^{(M)}|$.

Definition 3.1. For any bilinear tensor algorithm $\tilde{\Lambda}^{(s,t,v)}_{(D,K)}$, we denote its unique canonical bilinear algorithm as

$$\Lambda^{(F)} = \tilde{\Lambda}^{(s,t,v)}_{(D,K)},$$

where the unfoldings of $K$ into $F$ correspond to lexicographical orderings of the domains $D$.

The tensor domains of unique values are tailored for the symmetric tensor contraction algorithms (e.g. these domains are increasing integer sets for symmetric tensors). In Table 3.2, we give the particular values of $D$ and $K$ that yield the three tensor contraction algorithms considered in this paper. The bilinear rank of the direct evaluation algorithm is $\rank(\Psi^{(s,t,v)}_o) = \binom{n}{s} \binom{n}{t} \binom{n}{v}$, while the bilinear rank of the symmetry preserving algorithm is $\rank(\Phi^{(s,t,v)}_o) = \binom{n}{s} \binom{n}{t} \binom{n}{v}$.

| Table 3.1: Bilinear tensor algorithm domain and ranks for the three tensor contraction algorithms. |
|---------------------------------------------------------------|
| $\tilde{\Lambda}^{(s,t,v)}_{(D,K)}$ | $D^{(A)}$ | $D^{(B)}$ | $D^{(C)}$ | $D^{(M)}$ | $\rank(\tilde{\Lambda}^{(s,t,v)}_{(D,K)})$ |
| $\Upsilon^{(s,t,v)}$ | $[1,n]^{s+v}$ | $[1,n]^{v+t}$ | $[1,n]^{s+t}$ | $[1,n]^ω$ | $n^ω$ |
| $\Psi^{(s,t,v)}_o$ | $\leq [1,n]^{s+v}$ | $\leq [1,n]^{v+t}$ | $\leq [1,n]^{s+t}$ | $\leq [1,n]^ω$ | $\binom{n}{s} \binom{n}{t} \binom{n}{v}$ |
| $\Phi^{(s,t,v)}_o$ | $\leq [1,n]^{s+v}$ | $\leq [1,n]^{v+t}$ | $\leq [1,n]^{s+t}$ | $\leq [1,n]^ω$ | $\binom{n}{s} \binom{n}{t} \binom{n}{v}$ |

We will study the computation of subsets of products in bilinear algorithms. To achieve this, we define a subset of a bilinear algorithm to be a subset of columns in the matrix encoding.

Definition 3.2. We say a bilinear algorithm $\Lambda^{(G)}$ is a subset of bilinear algorithm $\Lambda^{(F)}$ (denoted $\Lambda^{(G)} \subseteq \Lambda^{(F)}$) if there exists a projection matrix $P ∈ \{0, 1\}^{\rank(\Lambda^{(G)}) × \rank(\Lambda^{(F)})}$ (with a single unit entry per column and at most one entry per row), such that

$$G^{(A)} = F^{(A)} P, \quad G^{(B)} = F^{(B)} P, \quad G^{(C)} = F^{(C)} P.$$

For tensor bilinear algorithms, $\tilde{\Lambda}^{(s,t,v)}_{(H,R)} \subseteq \tilde{\Lambda}^{(s,t,v)}_{(D,F)}$, when $\langle \tilde{\Lambda}^{(s,t,v)}_{(H,R)} \rangle \subseteq \langle \tilde{\Lambda}^{(s,t,v)}_{(D,F)} \rangle$.  


Table 3.2: Representations of three tensor contraction algorithms as bilinear tensor algorithms, $\hat{\Lambda}_{(D,K)}^{(s,t,v)}$. The last three columns give the non-zero fill structure of the tensors in $K$. To interpret $\chi$ and $\rho$ see Definition 2.9 and Definition 2.11 respectively. The new scaling factors given here for $\Phi_{D,K}^{(s,t,v)}$ arise due to multiple accumulations of tensor elements with repeating indices done within Algorithm 3.3.

| $\Psi_{D,K}^{(s,t,v)}$ | $\Phi_{D,K}^{(s,t,v)}$ |
|------------------------|------------------------|
| $\forall i \in [1,n]^s, j \in [1,n]^t, k \in [1,n]^v,$ | $\forall j \in [1,n]^s, i \in [1,n]^t, k \in [1,n]^v,$ |
| $\Psi_{D,K}^{(s,t,v)}$ | $\Phi_{D,K}^{(s,t,v)}$ |
| $\forall i \in [1,n]^s, j \in [1,n]^t, k \in [1,n]^v,$ | $\forall j \in [1,n]^s, i \in [1,n]^t, k \in [1,n]^v,$ |

4 Model of Execution and Costs

We present lower bounds for communication between main memory and cache on a sequential computer as well as communication between computers in the parallel setting. A communication cost is associated with a schedule of an execution DAG (directed acyclic graph) of an algorithm. In this section, we formally define execution DAGs for bilinear algorithms as well as how these executions are scheduled on sequential and parallel machine models. The cache size as well as the communication costs are implicitly parameterized by the tensor element size (all elements are assumed to be in the same ring $R$ and represented using a constant number of bits).

4.1 Execution Model for Bilinear Algorithms

Our definition of a bilinear algorithm allows for freedom in the implementation of the algorithm. In particular, it specifies only which linear combinations need to be computed, and not through what intermediates they are computed or in which order. We represent specific implementations via directed acyclic graphs (DAGs).

Definition 4.1. An execution DAG of a bilinear algorithm $\Lambda^{(F)}$, is a directed acyclic graph $G = (V,E)$. Each vertex in $V$ has either in-degree 0, in which case it corresponds to an input value, or in-degree 2, in which case it corresponds to the result of a (weighted) addition or a multiplication. Further, $V$ may be partitioned disjointly as

$$V = V^{(A)} \cup V^{(B)} \cup V^{(C)}.$$ 

The vertices in $V^{(A)}$ and $V^{(B)}$ correspond to linear combinations of $a$ and $b$ respectively, while the vertices in $V^{(C)}$ correspond to all computed bilinear forms (linear combinations of products). Vertices corresponding to inputs are denoted by $V^{(I)} \subseteq V^{(A)} \cup V^{(B)}$. Computed products (results of multiplication) and outputs are contained in $V^{(C)}$, we denote the computed products as $V^{(M)} \subseteq V^{(C)}$. We note that $\text{rank}(\Lambda^{(F)}) = |V^{(M)}|$. The set of edges $E$ may be partitioned disjointly as

$$E = E^{(A)} \cup E^{(B)} \cup E^{(AC)} \cup E^{(BC)} \cup E^{(C)}.$$ 

The parts $E^{(A)} \subset V^{(A)} \times V^{(A)}$ and $E^{(B)} \subset V^{(B)} \times V^{(B)}$ must contain binary trees which compute each linear combination of inputs to the products computed by $\Lambda^{(F)}$. The parts $E^{(AC)} \subseteq V^{(A)} \times V^{(M)}$ and $E^{(BC)} \subseteq V^{(B)} \times V^{(M)}$ define the inputs to each multiplication (so, if $\exists (v,w) \in E^{(AC)}, w \in V^{(M)}$ then $\exists (z,w) \in E^{(BC)}$ for some $z$). Finally, the part $E^{(C)} \subset V^{(C)} \times (V^{(C)} \setminus V^{(M)})$ encodes the summations that compute the output elements (subset of $V^{(C)}$).

To quantify the communication requirements of an execution DAG, it helps to reason about its expansion properties. Graph expansion is a known technique for derivation of communication lower bounds, which has previously been used for Strassen’s algorithm [3, 6, 19]. We employ a different but related notion of expansion, that is well-suited for bilinear algorithms. We seek to bound the size of the boundary of a subset of vertices of the execution DAG.
Definition 4.2. For execution DAG $G$ defined and partitioned as in Definition 4.1, we say that a subset of vertices that correspond to computed values, $Z \subset V \setminus V^{(f)}$ has

- **$A$-expansion** $c(A) = \zeta_A(G)(Z)$ if the number of external vertices in $V^{(A)}$ connected to $Z$ is $c(A)$,

$$
\zeta_A(G)(Z) := \{|v: (v, w) \in E, v \in V^{(A)} \setminus Z, w \in Z\},
$$

- **$B$-expansion** $c(B) = \zeta_B(G)(Z)$ if the number of external vertices in $V^{(B)}$ connected to $Z$ is $c(B)$,

$$
\zeta_B(G)(Z) := \{|v: (v, w) \in E, v \in V^{(B)} \setminus Z, w \in Z\},
$$

- **$C$-expansion** $c(C) = \zeta_C(G)(Z)$ if the number of vertices in $Z$ that are in $V^{(C)}$ or connected to a vertex in $V^{(C)} \setminus Z$ is $c(C)$ (these subsets may overlap),

$$
\zeta_C(G)(Z) := |Z \cap V^{(C)}| \cup \{w: (w, v) \in E, v \in V^{(C)} \setminus Z, w \in Z\}.
$$

$A$-expansion and $B$-expansion count vertices that are parts of the outer boundary of $Z$, while $C$-expansion counts vertices that are part of the inner boundary of $Z$. If an algorithm computes all the elements in $Z$, it must obtain inputs counted by $A$-expansion and $B$-expansion as well as yield outputs that are counted by $C$-expansion. We will use these notions of expansion to bound the number of inputs and outputs, and consequently the communication costs, associated with computing any subset of an execution DAG.

4.2 Sequential Schedule Cost Model

A sequential schedule imposes a total ordering on a (partially-ordered) execution DAG, interleaving the operations described by vertices in the execution DAG with reads from memory to cache, writes to cache from memory, and discards from cache. To measure the vertical communication cost on a sequential computer, we consider a cache of size $H$ elements and assume all data starts in main memory. We employ an idealized cache model, i.e. we do not consider track/cache-line size or mechanisms such as cache associativity. We assign reads and writes of data between main memory and cache unit communication cost. We do not pay attention to synchronization/latency cost.

We refer to this sequential machine model as $\mathfrak{N}(H)$. We do not restrict the size of the main memory of $\mathfrak{N}(H)$. We do not allow schedules executing on $\mathfrak{N}(H)$ to recompute any element computed by the algorithm. We assume none of the inputs of the algorithm reside in cache at the start of execution and that all of the outputs must be written to memory. We denote the sequential communication cost of a schedule executed on $\mathfrak{N}(H)$ as $Q$ and provide lower bounds for the cost on $Q$ for a given algorithm by considering all valid sequential schedules of this algorithm.

4.3 Parallel Schedule Cost Model

We also consider on a parallel schedules on a distributed-memory computer with a fully connected network. We denote this homogeneous parallel computer of $p$ processors as $\mathfrak{M}(p)$. We assume that each element of the input to the algorithm exists on a unique processor at the start of the execution of any parallel schedule and that the parallel schedule does not compute any element twice (no recomputation). We allow all processors to communicate with each other (fully connected network) on $\mathfrak{M}(p)$ via point-to-point messages. We measure the parallel horizontal communication cost $W$ of a schedule on $\mathfrak{M}(p)$ as the largest number of elements sent and received by any processor throughout the execution of the parallel schedule. Lower bounds on this simple communication metric yield lower bounds for LogP [9], LogGP [1], BSP [26], and the $\alpha$–$\beta$ critical path cost model (described in detail in [21]). In all of these models, the communication cost of a parallel schedule is at least the communication cost incurred by any given processor.

We assume throughout our analysis that the number of processors $p$ divides into the input/output domain sizes and the total number of operations. In our horizontal communication lower bounds, we treat $n$ (tensor dimension) and $p$ as asymptotic parameters, while assuming the tensor orders given by $s, t, v$ are constants.

**Definition 4.3.** We say a parallel schedule is **storage-balanced** if

- at the start of execution, each processor owns $x/p$ of the elements of each operand of size $x$.
• at the end of execution, each processor owns \( y/p \) of the elements of the output of size \( y \).

Storage-balanced schedules can have any initial distribution of inputs and final distribution of outputs, so long as it is minimal in memory usage at the start and end of execution, and each element is stored on a unique processor.

5 Lower Bounds for Bilinear Tensor Algorithms

In order to derive non-trivial lower bounds on the communication costs of a bilinear algorithm, we need to know something about the sparsity structure of the tensors in \( F \). In particular, we desire a lower bound on the number of inputs and outputs required by any subset of the products that the bilinear algorithm computes. Further, we want to know the minimal number of linear combinations that can represent the inputs and the outputs, motivating the use of matrix rank for our analysis.

Definition 5.1. A bilinear algorithm \( \Lambda^{(F)} \) has nondecreasing (in all variables) expansion bound \( E_\Lambda : \mathbb{N}^3 \rightarrow \mathbb{N} \), if for all \( \Lambda^{(R)} \subseteq \Lambda^{(F)} \),

\[
\text{rank}(\Lambda^{(R)}) \leq E_\Lambda \left( \text{rank}(R^{(A)}), \text{rank}(R^{(B)}), \text{rank}(R^{(C)}) \right).
\]

The expansion bound can be used to obtain lower bounds on the amount of communication needed to obtain the necessary inputs and produce the necessary outputs of an arbitrary set of computed products. The ranks of the matrices \( R^{(A)} \), \( R^{(B)} \), and \( R^{(C)} \) may be used to obtain lower bounds on the amount of input/output tensor data that is associated with computing the products.

Lemma 5.1. For execution DAG \( G = (V, E) \) (partitioned as in Definition 4.1) of bilinear algorithm \( \Lambda^{(F)} \), consider any computed subset \( Z \subseteq V \setminus V^{(I)} \). If \( \Lambda^{(F)} \) has expansion bound \( E_\Lambda \),

\[
|Z \cap V^{(M)}| \leq E_\Lambda(\zeta_G^{(A)}(Z), \zeta_G^{(B)}(Z), \zeta_G^{(C)}(Z)).
\]

Proof. Consider the bilinear algorithm subset \( \Lambda^{(R)} \subseteq \Lambda^{(F)} \), where the matrices in \( R \) contain the subset of columns of the matrices in \( F \) corresponding to the products \( H^{(M)} = Z \cap V^{(M)} \). By Definition 5.1, we must have

\[
|H^{(M)}| \leq E_\Lambda \left( \text{rank}(R^{(A)}), \text{rank}(R^{(B)}), \text{rank}(R^{(C)}) \right).
\]

Now, \( \zeta_G^{(A)}(Z) \) counts the number of linear combinations of elements in \( A \) on the boundary of \( Z \) within \( G \). All \( A \)-operands to products in \( H^{(M)} \) must be computed using these \( c^{(A)} \) linear combinations of \( A \) elements, \( v^{(A)} \). For any input vector \( a \) to \( \Lambda^{(R)} \), the \( A \)-operands of the products \( I^{(M)} \) must be \( w^{(A)} = R^{(A)} \cdot a \). Further, since \( v^{(A)} \) are linear combinations, there exists a matrix \( L \) such that, \( v^{(A)} = L \cdot a \) and since all products in \( H^{(M)} \) are computed from \( v^{(A)} \), there exists a matrix \( M \) such that \( w^{(A)} = M \cdot v^{(A)} = M \cdot L \cdot a \). Therefore, we must have \( \text{rank}(R^{(A)}) = \text{rank}(ML) \), and since \( \text{rank}(ML) \leq \text{rank}(M) \leq \zeta_G^{(A)}(Z) \), we have that \( \text{rank}(R^{(A)}) \leq \zeta_G^{(A)}(Z) \).

An identical argument may be made to show that \( \text{rank}(R^{(B)}) \leq \zeta_G^{(B)}(Z) \). The quantity \( \zeta_G^{(C)}(Z) \) is the number of output elements computed within \( Z \) and the number of bilinear forms within \( Z \) that are dependencies of output elements or other bilinear forms not included in \( Z \). Since the execution DAG may not recompute bilinear forms, by the same argument as for \( \zeta_G^{(A)}(Z) \), we assert that \( \text{rank}(R^{(C)}) \leq \zeta_G^{(C)}(Z) \). Otherwise the execution DAG may not be valid (the schedule cannot compute the result of the given transformation due to its rank). These rank bounds suffice to prove the theorem, as the expansion bound must be increasing.

5.1 Vertical Communication Lower Bounds for Bilinear Algorithms

Knowing the expansion bound of a bilinear algorithm allows us to obtain a vertical communication lower bound for it by a straightforward counting argument.

Theorem 5.2. Any load balanced schedule on \( \mathcal{R}(H) \) of any execution DAG, \( G = (V, E) \), of a bilinear algorithm \( \Lambda^{(F)} \) with \( \text{rank}(\Lambda^{(F)}) = r^{(A)}, \dim(\Lambda^{(F)}) = (r^{(A)}, r^{(B)}, r^{(C)}) \), and expansion bound \( E_\Lambda \) has vertical communication cost,

\[
Q_\Lambda(E_\Lambda, r^{(A)}, r^{(B)}, r^{(C)}, H) \geq \max \left[ \frac{2r^{(A)}H}{E_\Lambda^{\text{max}}(H)}, r^{(A)} + r^{(B)} + r^{(C)} \right],
\]

10
Proof. The second term in the maximum within the lower bound, \( r^{(A)} + r^{(B)} + r^{(C)} \), arises since any schedule must read all inputs into cache to operate on them and must write all outputs back to memory. Since we assumed that any bilinear algorithm is irreducible, \( r^{(A)} + r^{(B)} \) such inputs need to be read from memory and \( r^{(C)} \) outputs must be written back.

The first term in the maximum within the lower bound \( \frac{2k^{(A)}H}{E^\text{max}_X(H)} \), arises as a result of the expansion bound of the bilinear algorithm. Any load balanced schedule on \( \mathcal{H}(H) \) that computes \( \Lambda^{(X)} \) may be partitioned into \( f = \lfloor r^{(A)}/E^\text{max}_X(H) \rfloor \) intervals such that in each interval exactly \( E^\text{max}_X(H) \) products are computed and a last interval in which the remaining \( \bar{m} = r^{(A)} \mod E^\text{max}_X(H) \) forms are computed. In each of the first \( f \) intervals, if the set of computed vertices corresponding to products in the execution DAG is \( Z \subset V(M) \), by Lemma 5.1,

\[
E_\Lambda(\zeta_G^{(A)}(Z), \zeta_G^{(B)}(Z), \zeta_G^{(C)}(Z)) \geq |Z| = E^\text{max}_X(H).
\]

Furthermore, each of these schedule intervals requires \( \zeta_G^{(A)}(Z) \) linear combinations of \( A \) and \( \zeta_G^{(B)}(Z) \) linear combinations of \( B \) to be input, and \( \zeta_G^{(C)}(Z) \) linear combinations of products to be output. By the definition of \( E^\text{max}_X(H) \), we have \( \zeta_G^{(A)}(Z) + \zeta_G^{(B)}(Z) + \zeta_G^{(C)}(Z) \geq 3H \), so the total number of inputs and outputs for each of these intervals must be at least \( 3H \). Similarly, the last interval requires at least \( 3H \) inputs and outputs, where \( \bar{H} \) is the maximum integer such that \( E^\text{max}_X(H) \leq \bar{m} \). We additionally assert that

\[
\bar{H} \geq H(\bar{m}/E^\text{max}_X(H)),
\]

because \( \bar{m} \geq E^\text{max}_X(\bar{H}) \) and \( E^\text{max}_X(H)/E^\text{max}_X(\bar{H}) \geq H/\bar{H} \), the latter due to \( E^\text{max}_X \) being strictly increasing and convex.

Now, let \( x_i \) be the number of inputs present in cache prior to execution of interval \( i \) (by assumption no inputs start in cache so \( x_1 = 0 \)). The number of inputs present in cache at the end of execution of interval \( i \) should be equal to the number of inputs available for interval \( i+1 \), \( x_{i+1} \). Let the number of contributions to \( C \) (bilinear forms), which remain in cache (are not written to memory) at the end of interval \( i \), be \( y_i \). The rest of the outputs produced by interval \( i \) must be written to memory. Let \( x_{f+1} \) be the number of inputs in cache prior to execution of the last interval, by assumption all outputs must be written to memory by the end of this interval, so \( x_{f+1} = 0 \). In total, the amount of reads from memory and writes to memory done during the execution of interval \( i \) with \( E^\text{max}_X \) products is then at least \( w_i \geq 3H - x_i - y_i, \forall i \in [1,f] \) and \( w_{f+1} \geq 3\bar{H} - x_{f+1} \). Now, since the inputs and outputs which are kept in cache at the end of interval \( i \) must fit in cache, we know that \( \forall i \in [1,f], x_{i+1} + y_i \leq \bar{H} \). Rearranging this and substituting \( y_i \) into our bound on reads and writes, we obtain \( w_i \geq 2H - x_i + x_{i+1}, \forall i \in [1,f] \). Summing over all intervals and extracting the first interval to apply \( x_1 = 0 \) yields the desired lower bound on total communication cost,

\[
Q_\Lambda(E_\Lambda, r^{(A)}, r^{(B)}, r^{(C)}, H) \geq \sum_{i=1}^{f+1} w_i \geq 2H + x_1 + \sum_{i=2}^{f} (2H - x_i + x_{i+1}) + 3\bar{H} - x_{f+1}
\]

\[
= 2fH + 3\bar{H} \geq 2H \left\lceil r^{(A)}/E^\text{max}_X(H) \right\rceil + 3H(\bar{m}/E^\text{max}_X(H)) \geq \frac{2k^{(A)}H}{E^\text{max}_X(H)}.
\]

\[\square\]

This vertical communication lower bound implies that, aside from moving the inputs and outputs between memory and cache, any execution of the bilinear algorithm requires additional communication that is dependent on its bilinear expansion. In particular, a bilinear expansion lower bound can be maximized to bound above the number of products that can be computed given any set of elements that fits in cache. Such an upper bound consequently yields the lower bound on communication with respect to the total amount of products computed.

5.2 Horizontal Communication Lower Bounds for Bilinear Algorithms

We can also formulate a lower bound on horizontal communication cost based on the expansion rate and the dimensions of the inputs.
Theorem 5.3. Any load balanced schedule on $\mathcal{M}(p)$ of any execution DAG of a bilinear algorithm $\Lambda^{(F)}$ with $\text{rank}(\Lambda^{(F)}) = r(\Lambda)$, $\dim(\Lambda^{(F)}) = (r(A), r(B), r(C))$, and expansion bound $\mathcal{E}_\Lambda$ has horizontal communication cost,

$$W_\Lambda(\mathcal{E}_\Lambda, r(A), r(A), r(B), r(C), p) \geq c(A) + c(B) + c(C)$$

for some non-negative $c(A), c(B), c(C) \in \mathbb{N}$ such that

$$r(A)/p \leq \mathcal{E}_\Lambda(c(A) + r(A)/p, c(B) + r(B)/p, c(C) + r(C)/p).$$

Proof. For any execution DAG $G = (V, E)$ of $\Lambda^{(F)}$, at least one processor must compute more than $r(A)/p$ products. Let $Z \subset V \setminus V^E$ be the set of all linear combinations of elements of $A$ and $B$ and bilinear forms this processor computes, so $|Z \cap V^E| \geq r(A)/p$. The $A$- and $B$- expansions of $Z$ count all linear combinations of input elements that are operands of products or additions computed by the processor, but are not themselves computed by this processor. Such linear combinations must either be input initially or received via a message. The $C$-expansion counts all bilinear forms computed by this processor that are outputs or operands to sums computed by other processors. Such bilinear forms must be output or sent in an outgoing message by this processor. By Lemma 5.1, we can relate the number of products computed by this processor to these expansion set sizes. In particular, if for the processor computing vertices $Z$,

- the $A$-expansion (inputs or received elements) is $d(A)$,
- the $B$-expansion (inputs or received elements) is $d(B)$,
- the $C$-expansion (outputs or sent elements) is $d(C)$,

then $r(A)/p \leq \mathcal{E}_\Lambda(d(A), d(B), d(C))$.

Now, since we assume schedules on $\mathcal{M}(p)$ must have load-balanced inputs and outputs, this processor owns $r(A)/p$ elements of $A$ and $r(B)/p$ elements of $B$ at the start of execution, and outputs $r(C)/p$ elements of $C$. Thus, the processor computing $Z$ must receive at least $c(A) = d(A) - r(A)/p$ linear combinations of elements of $A$, and at least $c(B) = d(B) - r(B)/p$ linear combinations of elements of $B$. Further, it outputs $r(C)/p$ elements of $C$, so it must send at least $c(C) = d(C) - r(C)/p$ bilinear forms. Thus, for some $c(A), c(B), c(C) \in \mathbb{N}$, we have

$$r(A)/p \leq \mathcal{E}_\Lambda(d(A), d(B), d(C)) = \mathcal{E}_\Lambda(c(A) + r(A)/p, c(B) + r(B)/p, c(C) + r(C)/p),$$

with a corresponding lower bound on communication cost lower bound of

$$W_\Lambda(\mathcal{E}_\Lambda, r(A), r(A), r(B), r(C), p) \geq c(A) + c(B) + c(C).$$

This horizontal communication lower bound expresses the minimum amount of data that needs to be communicated $(c(A) + c(B) + c(C))$, given that each processor starts with a set amount of inputs $(r(A)/p$ and $r(B)/p)$ and ends a set amount of outputs $(r(C)/p)$. The amount of communication depends on the rank as well as the expansion of the bilinear algorithm.

6 Volumetric Inequalities

To derive expansion bounds for algorithms, we will employ volumetric inequalities to lower bound the sizes of sets of projections. The lower bounds in this section are based on the generalized Loomis-Whitney inequality [15, 25].

Theorem 6.1. Let $V$ be a set of $m$-tuples, $V \subseteq [1, n]^m$. Consider $(m)$ projections:

$$\forall \vec{s} \in [1, m]^r, \quad \pi_{\vec{s}}(\vec{i}) := (i_{s_1}, \ldots, i_{s_r}),$$

and apply these projections to all elements in $V$ to form the projection sets:

$$\forall \vec{s} \in [1, m]^r, \quad L_{\vec{s}} := \{\pi_{\vec{s}}(\vec{i}) : \vec{i} \in V\}.$$ 

The cardinality of the set $V$ may be upper bound by the cardinalities of these projections,

$$|V| \leq \left( \prod_{\vec{s} \in [1, m]^r} |L_{\vec{s}}| \right)^{1/\binom{m}{r-1}}.$$
The standard Loomis-Whitney inequality [15] is given by Theorem 6.1 with \( m = d \) and \( r = d - 1 \). We use the \( d = 3 \) form of it to prove Lemma 7.1.

When applying such inequalities to obtain communication lower bounds, we are generally interested in a lower bound on the size of the projected sets \( \{ L_g \} \), rather than an upper bound on \( V \). So, we introduce the following lemma, which gives a lower bound on the union of the projections \( L = \bigcup_{g \in \mathbb{G}} L_g \) and can be succinctly expressed using \( \chi^r \) (Definition 2.10).

**Lemma 6.2.** Let \( V \) be a set of \( m \)-tuples, \( V \subseteq [1, n]^m \), consider the projected sets given by the projection map \( \chi^r \),

\[
L = \{ \bar{w} : \bar{w} \in \chi^r(\bar{v}), \bar{v} \in V \},
\]

then we have \( |V| \leq |L|^{m/r} \).

The proof of Lemma 6.2 may be easily obtained directly from Theorem 6.1, see [20].

## 7 Lower Bounds for Nonsymmetric Contraction Algorithms

We exercise the bilinear algorithm lower bound infrastructure by deriving communication lower bounds for nonsymmetric contractions (matrix multiplication and the general case, which follows trivially). These results are well-known, although our lower bound constants are stronger than those presented in previous analyses. All later communication lower bound proofs will follow the same logical structure as the ones in these section.

### 7.1 Lower Bounds for Matrix Multiplication

We start by applying the theory developed for bilinear algorithms to matrix multiplication, reproducing known results. As for all bilinear algorithms, we start by deriving the expansion bound of the algorithm, then applying Theorem 5.2 and Theorem 5.3 to obtain horizontal and communication lower bounds, respectively.

**Lemma 7.1.** An expansion bound (Definition 5.1) on the classical (non-Strassen-like) matrix multiplication algorithm of \( m \)-by-\( k \) matrix \( A \) with \( k \)-by-\( n \) matrix \( B \) into \( m \)-by-\( n \) matrix \( C \) is

\[
\mathcal{E}_{MM}(d(A), d(B), d(C)) = (d(A)d(B)d(C))^{1/2}.
\]

**Proof.** For the matrix multiplication bilinear tensor algorithm \( \hat{A}_{\{1,1,1\},D,K} \), where \( D(A) = [1, m][1, k], D(B) = [1, k][1, n], D(C) = [1, m][1, n][1, k], \) and \( D(M) = [1, m][1, n][1, k] \) (these compose \( D \)), the sparse tensors specifying the corresponding bilinear algorithm are

\[
\forall i_1 \in [1, m], i_2 \in [1, n], i_3 \in [1, k], \quad K_{1i_1i_2i_3}^{(A)} = 1, \quad K_{1i_1i_2i_3}^{(B)} = 1, \quad K_{1i_1i_2i_3}^{(C)} = 1.
\]

Consider any \( A^{(\mathbb{R})} \subseteq \hat{A}_{\{1,1,1\},D,K} \) and the associated subset of products, \( V \subseteq D^{(M)} \). The columns of the matrices \( R^{(A)}, R^{(B)}, \) and \( R^{(C)} \) (contained in \( \mathbb{R} \) each have a single non-zero (unit) entry and so are only linearly dependent when they are equivalent. Let the numbers of unique columns in these three matrices be \( d(A) = \text{rank}(R^{(A)}), d(B) = \text{rank}(R^{(B)}), \) and \( d(C) = \text{rank}(R^{(C)}). \) The number of such unique columns is also the size of the projection sets \( d(A) = |L_{(1,3)}| \), where \( L_{(1,3)} = \{ (i_1,i_3) : (i_1,i_2,i_3) \in V \} \) and similarly for \( B \) and \( C \). Therefore, we can apply Theorem 6.1 with \( m = 2 \) and \( r = 3 \) to bound the cardinality of \( V \) as

\[
\text{rank}(A^{(\mathbb{R})}) = |V| \leq (d(A)d(B)d(C))^{1/2} = (\text{rank}(R^{(A)}) \text{rank}(R^{(B)}) \text{rank}(R^{(C)}))^{1/2}.
\]

Thus Definition 5.1 is satisfied for the expansion bound \( E_{MM} \).

We now give a lower bound on the communication cost of matrix multiplication. This lower bound result is not new from an asymptotic stand-point (the asymptotic lower bound was first proven by [12]). The first term in the bound is a factor of 16 higher than the lower bound given earlier by [2], where the assumptions on initial/final data layout and overlap between input entries were looser.
Theorem 7.2. Any load balanced sequential schedule of the classical (non-Strassen-like) matrix multiplication algorithm of $m$-by-$k$ matrix $A$ with $k$-by-$n$ matrix $B$ into $m$-by-$n$ matrix $C$ on $\Omega(H)$ has vertical communication cost,

$$Q_{MM}(m, n, k, H) \geq \max \left[ \frac{2mnk}{\sqrt{H}}, mk + kn + mn \right].$$

Proof. By Lemma 7.1, the classical matrix multiplication algorithm has expansion bound $E_{MM}(d(A), d(B), d(C)) = (d(A)d(B)d(C))^{1/2}$. Applying Theorem 5.2, with this expansion bound, we obtain the communication lower bound,

$$Q_{MM}(m, n, k, H) \geq \max \left[ \frac{2mnkH}{E_{MM}^\max(H)}, mk + kn + mn \right],$$

where

$$E_{MM}^\max(H) = \max_{c(A), c(B), c(C) \in \mathbb{N}, c(A) + c(B) + c(C) \leq 3H} \left( c(A)c(B)c(C) \right)^{1/2} = H^{3/2},$$

which is strictly increasing and convex for $H \geq 1$ as needed, so we arrive at the bound stated in the theorem.

The following lower bound, Theorem 7.3 was proven in [10]. We give an alternate proof using Theorem 5.3.

Theorem 7.3. Any storage-balanced schedule of the classical (non-Strassen-like) matrix multiplication algorithm of $m$-by-$k$ matrix $A$ with $k$-by-$n$ matrix $B$ into $m$-by-$n$ matrix $C$ on $\Omega(p)$ has horizontal communication cost,

$$W_{MM}(m, n, k, p) = \Omega\left( W_O(\min(m, n, k), \text{median}(m, n, k), \max(m, n, k), p) \right),$$

where

$$W_O(x, y, z, p) = \begin{cases} 
\left( \frac{xyz}{p} \right)^{2/3} & : p > yz/x^2, \\
\left( \frac{yz}{p} \right)^{1/2} & : yz/x^2 \geq p > z/y, \\
x/y & : z/y \geq p.
\end{cases}$$

Proof. By Lemma 7.1, the classical matrix multiplication algorithm has expansion bound $E_{MM}(d(A), d(B), d(C)) = (d(A)d(B)d(C))^{1/2}$. Applying Theorem 5.3, with this expansion bound, we obtain the bound,

$$W_{MM}(m, n, k, p) \geq d(A) + d(B) + d(C),$$

for some $d(A), d(B), d(C) \in \mathbb{N}$ such that

$$mnk/p \leq [(d(A) + mk/p)(d(B) + kn/p)(d(C) + mn/p)]^{1/2}.$$  

Letting $x = \min(m, n, k)$, $y = \text{median}(m, n, k)$, and $z = \max(m, n, k)$, we rewrite the above as

$$W_O(x, y, z, p) = d_1 + d_2 + d_3,$$

for some $d_1, d_2, d_3 \in \mathbb{N}$ such that

$$xyz/p \leq [(d_1 + xy/p)(d_2 + xz/p)(d_3 + yz/p)]^{1/2}.$$  

The symmetry of the objective and constraint in $d_1, d_2, d_3$ tells us that due to $x \leq y \leq z$, the optimal solution must have $d_1 \geq d_2 \geq d_3$. Asymptotically, there are three scenarios that are distinguished by which term in the right-hand side of the constraint is greatest (dominant):

- $\sqrt{d_1 d_2 d_3}$ is the dominant term, implies $W_O(x, y, z, p) = \Omega((xyz/p)^{2/3})$.
- $\sqrt{d_1 d_2 yz/p}$ is the dominant term, implies $W_O(x, y, z, p) = \Omega(x \sqrt{yz/p})$.
- $(z/p)^{\sqrt{d_1 xy}}$ is the dominant term, implies $W_O(x, y, z, p) = \Omega(xy)$.

Computing the ranges in which each of these three terms implies the least communication yields the lower bounds given in the theorem.

These matrix multiplication lower bounds can be interpreted geometrically. They correspond to partitioning the cube of $mnk$ products in matrix multiplication in one, two, or three dimensions (1D, 2D, and 3D algorithms).
7.2 Lower Bounds for Nonsymmetric Contractions

We now introduce communication lower bounds for the nonsymmetric contraction algorithm. As we explained after the statement of Algorithm 3.1, \( \Upsilon^{(s,t,v)}(A, B) \) is equivalent to a matrix multiplication of an \( n^s \times n^t \) matrix with an \( n^v \times n^t \) matrix yielding a \( n^v \times n^t \) matrix. Therefore, its communication lower bounds have a direct correspondence to those of matrix multiplication.

**Theorem 7.4.** Any schedule of \( \Upsilon^{(s,t,v)}(A, B) \) on \( \mathcal{M}(H) \) has vertical communication cost,

\[
Q_T(n, s, t, v, H) \geq \max \left[ \frac{2n^w}{\sqrt{H}}, n^{s+t} + n^{s+v} + n^{v+t} \right].
\]

**Proof.** Since any matrix multiplication may be expressed as a direct evaluation nonsymmetric contraction algorithm, the communication cost of this nonsymmetric contraction algorithm cannot be lower than the optimal communication cost of the standard matrix multiplication algorithm that evaluates the \( n^w \) products directly. Therefore, \( Q_T(n, s, t, v, H) \geq Q_{MM}(n^s, n^t, n^v, H) \), which yields the lower bound above. \( \blacksquare \)

Similarly, we obtain a bound for horizontal communication cost below.

**Theorem 7.5.** Any storage-balanced schedule of \( \Upsilon^{(s,t,v)}(A, B) \) on \( \mathcal{M}(p) \) has horizontal communication cost,

\[
W_T(n, s, t, v, p) = \Omega \left( W_{MM}(n^s, n^t, n^v, p) \right).
\]

**Proof.** By the same argument as in the proof of Theorem 7.4, this algorithm can be used to perform a matrix multiplication with dimensions \( n^s, n^t, \) and \( n^v \), hence the bound stated in the theorem. \( \blacksquare \)

8 Lower Bounds for Direct Evaluation of Symmetric Contractions

We apply a similar lower bound approach for the direct evaluation algorithm of symmetric tensor contractions and obtain communication lower bounds that are somewhat smaller than the nonsymmetric case. This result is expected, since the direct evaluation algorithm requires less computation than the nonsymmetric algorithm for most contractions. However, for matrix-vector-like contractions, we also provide an additional expansion bound for the direct evaluation algorithm that does not have a counterpart for the nonsymmetric algorithm. We start by deriving a matrix-multiplication-like expansion bound for this bilinear algorithm.

**Lemma 8.1.** An expansion bound on \( \Psi_o^{(s,t,v)} \) with \( q := \left[ \begin{pmatrix} s^+ v^+ \\ t \end{pmatrix} \right] \) is

\[
E_{\Psi}^{(s,t,v)}(d(A), d(B), d(C)) = q \left( d(A) d(B) d(C) \right)^{1/2}
\]

**Proof.** For the bilinear tensor algorithm \( \hat{\Lambda}_{(D,K)}^{(s,t,v)} = \Psi_o^{(s,t,v)} \), the products are specified by the following sparse tensors:

\[
\forall \vec{g} \in [1, n]^{s+v}, \vec{I} \in [1, n]^t, (\vec{j}, \vec{k}) \in \chi_v^s(\vec{g}), \quad R^{(A)}_{gijkl} = 1,
\]

\[
\forall \vec{h} \in [1, n]^{v+t}, \vec{j} \in [1, n]^s, (\vec{k}, \vec{i}) \in \chi_v^t(\vec{h}), \quad R^{(B)}_{hijkl} = 1,
\]

\[
\forall \vec{i} \in [1, n]^{s+t}, \vec{k} \in [1, n]^v, (\vec{j}, \vec{l}) \in \chi_v^t(\vec{i}), \quad R^{(C)}_{ijkl} = s! t! \rho(\vec{k})
\]

Consider any \( \Lambda^{(R)} \subseteq \hat{\Lambda}_{(D,K)}^{(s,t,v)} \) and the associated subset of products \( V \subseteq D^{(M)} = [1, n]^s \times [1, n]^t \times [1, n]^v \). Like in matrix multiplication, the columns of the matrices \( R^{(A)}, R^{(B)}, \) and \( R^{(C)} \) (with elements contained in \( R \) each have a single non-zero entry (as each product has one operand from \( A \), one from \( B \) and contributes to one output in \( C \)) and so are only linearly dependent when they are equivalent. Consider the three projections:

\[
L_{(1,3)} = \{ \vec{jk} : \vec{jk} \in V \}, \quad L_{(2,3)} = \{ \vec{ji} : \vec{ji} \in V \}, \quad L_{(1,2)} = \{ \vec{ji} : \vec{ji} \in V \}
\]

The row corresponding to index \( \vec{g} \in [1, n]^{s+v} \) is non-zero in \( R^{(A)} \) if \( \exists \vec{k} \in L_{(1,3)} \) such that \( (\vec{j}, \vec{k}) \in \chi_v^s(\vec{g}) \). Since there is a unique such row \( \vec{g} \) for each entry of \( L_{(1,3)} \) and \( |\chi_v^s(\vec{g})| = (s+v) \), it follows that the number of non-zero rows
in $R^{(A)}$ must be at least $d(A) := \text{rank}(R^{(A)}) \geq |L_{(1,3)}|/(s+v)$. Similarly for $B$ and $C$ with $d(B) := \text{rank}(R^{(B)}) \geq |L_{(2,3)}|/(t+v)$ and $d(C) := \text{rank}(R^{(C)}) \geq |L_{(1,2)}|/(s+t)$. By Theorem 6.1 with $m = 2$ and $r = 3$, we then obtain

$$|V| \leq (|L_{(1,2)}||L_{(1,3)}||L_{(2,3)}|)^{1/2} \leq \left( \binom{s+v}{v} d(A) \binom{t+v}{t} d(B) \binom{s+t}{s} d(C) \right)^{1/2},$$

so Definition 5.1 is satisfied for the expansion bound,

$$E_{\Psi}^{(s,t,v)}(d(A), d(B), d(C)) = q \left( d(A) d(B) d(C) \right)^{1/2},$$

where $q = \left[ \binom{s+v}{v} \binom{t+v}{t} \binom{s+t}{s} \right]^{1/2}$.

We now also derive an additional expansion bound for the direct evaluation algorithm for symmetric contractions. This bound is valid when exactly one of $s, t, v$ is zero (the contraction is matrix-vector-like), and in some cases can be stronger than the matrix-multiplication-like bound above. We will use it to prove a horizontal communication lower bound in Theorem 8.5.

**Lemma 8.2.** An expansion bound on $\Psi_{\circ}^{(s,t,v)}$ when exactly one of $s, t, v$ is zero is

$$E_{\Psi}^{(s,t,v)}(d(A), d(B), d(C)) = \left( \binom{\omega}{\min(s,v)} - 1 \right) d(A) + \left( \binom{\omega}{\min(v,t)} - 1 \right) d(B) + \left( \binom{\omega}{\min(s,t)} - 1 \right) d(C) + \min \left( (d(A))^{\omega/(s+v)}, (d(B))^{\omega/(v+t)}, (d(C))^{\omega/(s+t)} \right).$$

**Proof.** Let $\Lambda_{(s,t,v)} = \Psi_{\circ}^{(s,t,v)}$. We prove the case when $v = 0$ (the other two are similar). Consider any $\Lambda^{(R)} \subseteq \Lambda_{(s,t,v)}$ and the associated subset of products, $V \subseteq D^{(M)} = \subseteq [1, n]^s \subseteq [1, n]^t$. Let $c_1$ be the number of rows of $R^{(C)}$ that contain $\binom{\omega}{s}$ nonzeros. Let $c_2$ be the number of other nonzero rows of $R^{(C)}$ (that contain at least one and at most $\binom{\omega}{s} - 1$ nonzeros). Since, when $v = 0$, each column in $R^{(C)}$ has a single nonzero, $d(C) := \text{rank}(R^{(C)}) = c_1 + c_2$, and further,

$$|V| \leq \left( \binom{\omega}{s} - 1 \right) c_1 + \left( \binom{\omega}{s} - 1 \right) d(C) + c_1.$$

Let $Z \subseteq \subseteq [1, n]^\omega$ be the set of indices of the $c_1$ rows (C entries) with $\binom{\omega}{s}$ nonzeros. Since the bilinear algorithm subset computes all products contributing to these $c_1$ rows, its $R^{(A)}$ and $R^{(B)}$ matrices have nonzeros in all rows which correspond to entries of $A$ and $B$ contributing to these $c_1$ entries of $C$. Therefore, the set of rows with nonzeros in $R^{(A)}$ is

$$L^{(A)} = \{ \vec{i} : \vec{i} \in \chi^* \vec{i} \in Z \}.$$

Since each column of $R^{(A)}$ has a single nonzero, any set of unique rows is linearly independent, which implies that the rank of $R^{(A)}$ is at least $|L^{(A)}|$. By Lemma 6.2, $|L^{(A)}| \geq |Z|^s/\omega$, so $d(A) \geq |Z|^s/\omega = c_1^{s/\omega}$. By a similar argument, the rank of $R^{(B)}$ is at least $d(B) \geq c_1^{t/\omega}$.

Therefore, since $c_1 \leq \min \left( (d(A))^{\omega/s}, (d(B))^{\omega/t}, d(C) \right)$, given any subset bilinear algorithm where the ranks of $R^{(A)}, R^{(B)},$ and $R^{(C)}$ being $d(A), d(B),$ and $d(C)$, respectively, we can bound the rank of the subset bilinear algorithm by the formula,

$$E_{\Psi}^{(s,t,0)}(d(A), d(B), d(C)) = \left( \binom{\omega}{s} - 1 \right) d(C) + \min \left( (d(A))^{\omega/s}, (d(B))^{\omega/t}, d(C) \right).$$

Further, there are symmetric bounds for other permutations of $s, t, v$,

$$E_{\Psi}^{(0,t,v)}(d(A), d(B), d(C)) = \left( \binom{\omega}{t} - 1 \right) d(B) + \min \left( (d(A))^{\omega/v}, (d(B))^{\omega/t}, (d(C))^{\omega/t} \right),$$

$$E_{\Psi}^{(s,0,v)}(d(A), d(B), d(C)) = \left( \binom{\omega}{s} - 1 \right) d(A) + \min \left( (d(A))^{\omega/s}, (d(B))^{\omega/v}, (d(C))^{\omega/s} \right).$$
We can generalize the second term in all of these bounds by
\[
\min \left( \left( d(A)^\omega/(s+v) \right), \left( d(B)^\omega/(v+t) \right), \left( d(C)^\omega/(s+t) \right) \right),
\]
so long as exactly one of \( s, t, v \) is zero. We can similarly generalize the first term in each of the three bounds, yielding the bound in the lemma.

\[\square\]

### 8.1 Vertical Communication Lower Bounds for Direct Evaluation of Symmetric Contractions

We have shown that the expansion bound of the direct evaluation algorithm for symmetric contractions is larger than that of classical matrix multiplication (nonsymmetric contractions) by a constant factor. Accordingly, the communication lower bounds are lower by an associated factor. A simple example of when less communication is needed for the symmetric contraction algorithm than the nonsymmetric one, is when all tensors fit into cache. In this case, it suffices to read each element of \( A \) and \( B \) once and write each element of \( C \) once, which attains the below lower bound when \( s = t = v \) and is more efficient than the respective matrix multiplication.

**Theorem 8.3.** Any storage-balanced sequential schedule of \( \Psi^{(s,t,v)}(A, B) \) on \( \mathcal{H} \) has vertical communication cost,
\[
Q\psi(n, s, t, v, H) \geq \max \left[ \frac{\binom{n}{s} \binom{n}{t} \binom{n}{v}}{q\sqrt{H}}, \left( \binom{n}{s+v} \right), \left( \binom{n}{v+t} \right), \left( \binom{n}{s+t} \right) \right],
\]
where \( q = \left[ \left( \binom{s+v}{s} \right)^{1/2} \cdot \left( \binom{v+t}{v} \right)^{1/2} \right]. \)

**Proof.** By lemma 8.1, we know that
\[
\mathcal{E}_{\psi}^{(s,t,v)}(q(A), q(B), q(C)) = q \left( d(A)^{\omega/(s+v)} d(B)^{\omega/(v+t)} d(C)^{\omega/(s+t)} \right)^{1/2}.
\]
Applying Theorem 5.2, with this expansion bound, we obtain the communication lower bound,
\[
Q\psi(n, s, t, v, H) \geq \max \left[ \frac{\binom{n}{s} \binom{n}{t} \binom{n}{v}}{\mathcal{E}_{\psi}^{\text{max}}(H)}, \left( \binom{n}{s+v} \right), \left( \binom{n}{v+t} \right), \left( \binom{n}{s+t} \right) \right],
\]
where
\[
\mathcal{E}_{\psi}^{\text{max}}(H) = \max_{c(A), c(B), c(C) \in N, c(A) + c(B) + c(C) \leq 3H} q(c(A))^{1/2} c(B)^{1/2} c(C)^{1/2}.
\]
which is strictly increasing and convex for \( H \geq 1 \) as needed.

\[\square\]

### 8.2 Horizontal Communication Lower Bounds for Direct Evaluation of Symmetric Contractions

For horizontal communication cost, we again start by showing that the matrix multiplication lower bound extends to the direct evaluation algorithm for symmetric contractions.

**Theorem 8.4.** Any storage-balanced schedule of \( \Psi^{(s,t,v)}(A, B) \) on \( \mathcal{P} \) has horizontal communication cost,
\[
W\psi(n, s, t, v, p) = \Omega \left( W\omega(\min(n, s, t, v), \max(n, s, t, v), p) \right),
\]
where \( W\omega \) is the same as given in Theorem 7.3,
\[
W\omega(n^x, n^y, n^z, p) = \begin{cases} 
\left( \frac{n^{x+y+z}}{p} \right)^{2/3} & : p > n^{y+z-2x}, \\
\left( \frac{n^{y+z}}{p} \right)^{1/2} & : n^{y+z} \geq p > n^{z-y}, \\
\left( \frac{n^{z-y}}{p} \right) & : n^{z-y} \geq p.
\end{cases}
\]
Proof. By Lemma 8.1, we have the expansion bound
\[ E^{(s,t,v)}_\Psi(d^{(A)}, d^{(B)}, d^{(C)}) = q(d^{(A)} d^{(B)} d^{(C)})^{1/2} \]
Applying Theorem 5.3, with this expansion bound, we obtain the bound,
\[ W_\Psi(n, s, t, v, p) \geq d^{(A)} + d^{(B)} + d^{(C)} \]
for some \( d^{(A)}, d^{(B)}, d^{(C)} \in \mathbb{N} \) such that
\[ \frac{\binom{n}{s} \binom{n}{t} \binom{n}{v}}{p} \leq q \left[ \left( d^{(A)} + \binom{n}{s+v}/p \right) \left( d^{(B)} + \binom{n}{v+t}/p \right) \left( d^{(C)} + \binom{n}{s+t}/p \right) \right]^{1/2}. \]
This bound is very similar to what we encountered for matrix multiplication in the proof of Theorem 7.3, so we proceed accordingly. Let \( x = \min(s, t, v) \), \( y = \text{median}(s, t, v) \), and \( z = \max(s, t, v) \), so that \( x \leq y \leq z \) and rewrite the above objective function as
\[ W_O(n^x, n^y, n^z, p) \geq d_1 + d_2 + d_3, \]
and constraint function as
\[ \frac{\binom{n}{x} \binom{n}{y} \binom{n}{z}}{p} \leq q \left[ \left( d_1 + \binom{n}{x+y}/p \right) \left( d_2 + \binom{n}{x+z}/p \right) \left( d_3 + \binom{n}{y+z}/p \right) \right]^{1/2}. \]
When \( x, y, z > 0 \), we again have three possible asymptotically dominant terms in the optimal solution,
- \( q\sqrt{d_1 d_2 d_3} \) is the dominant term, implies \( W_O(n^x, n^y, n^z, p) = \Omega((n^{x+y+z}/p)^{2/3}) \),
- \( q\sqrt{d_1 d_2 n^{y+z}}/p \) is the dominant term, implies \( W_O(n^x, n^y, n^z, p) = \Omega(n^{x+y+z}/p) \),
- \( q(n^z/p)\sqrt{d_1 n^{x+y}} \) is the dominant term, implies \( W_O(n^x, n^y, n^z, p) = \Omega(n^{x+y}) \).

In the parallel case we derive an additional horizontal communication lower bound for matrix-vector-like contractions. The additional bound is stronger than the bound obtained via the reduction from matrix multiplication when \( s, t, v \) are all unequal (and one is zero). In the sequential scenario, the communication cost of such cases is dominated by reading the inputs from memory to cache or writing the output to memory. In the parallel scenario, the largest tensor can be kept in place, so communication of the second-largest tensor must be considered.

When \( v = 0 \), the new communication lower bound then arises as a consequence of symmetrization needed to compute \( C \). When \( s = 0 \) or \( t = 0 \), this bound is a consequence of the assumption that each unique elements of the largest the symmetric operand is stored on a unique processor. This assumption corresponds to a ‘packed’ distributed layout [23] for symmetric tensors. Therefore, using an ‘unpacked’ layout, where the tensor operands are stored as if they were nonsymmetric, would make it possible to have asymptotically lower communication costs in cases when either \( s \) or \( t \) is zero and \( v \neq s \) as well as \( v \neq t \).

Theorem 8.5. When exactly one of \( s, t, v \) is zero, any storage-balanced schedule of \( \Psi^{(s,t,v)}_{\omega}(A, B) \) on \( \mathcal{M}(p) \) has horizontal communication cost,
\[ W_\Psi(n, s, t, v, p) = \Omega \left( (n^\omega / p)^{\max(s,t,v)} / \omega \right). \]

Proof. When \( v = 0 \), by Lemma 8.2, we have the expansion bound
\[ E^{(s,t,0)}_\Psi(d^{(A)}, d^{(B)}, d^{(C)}) = \binom{\omega}{s} - 1 \right) d^{(C)} + \min \left( \left( d^{(A)} \right)^{\omega/s}, \left( d^{(B)} \right)^{\omega/t}, \left( d^{(C)} \right)^{\omega/t} \right). \]
Applying Theorem 5.3, we obtain
\[ W_\Psi(n, s, t, 0, p) \geq d^{(A)} + d^{(B)} + d^{(C)}, \]
for some \( d^{(A)}, d^{(B)}, d^{(C)} \in \mathbb{N} \) such that
\[ \frac{\binom{n}{s} \binom{n}{t} \binom{n}{v}}{p} \leq \left( \binom{n}{s} - 1 \right) d^{(C)} + \left( \binom{n}{\omega} / p \right) \]
\[ + \min \left( \left( d^{(A)} \right)^{\omega/s}, \left( d^{(B)} \right)^{\omega/t}, \left( d^{(C)} \right)^{\omega/t} \right). \]
Using the fact that \( \binom{n}{\omega} \leq \binom{\omega}{\omega} \binom{n}{\omega} \), we can simplify the above constraint to
\[
\frac{\binom{n}{\omega}}{p} \leq \left( \left( \frac{\omega}{s} - 1 \right) d(C) + \min \left[ \left( \frac{d(A) + \frac{\binom{n}{\omega}}{p}}{\omega} \right)^{\omega/s}, \left( \frac{d(B) + \frac{\binom{n}{\omega}}{p}}{\omega} \right)^{\omega/t}, d(C) + \frac{\binom{n}{\omega}}{p} \right] \right).
\]
If the first term in the right hand side equation is greater than the min, we have \( d(C) = \Omega(n^\omega/p) \), and the theorem holds, since \( W_\Psi(n, s, t, v, p) \geq d(C) \). If the min is greatest, we have
\[
d(A) = \Omega \left( \left( \frac{n^\omega}{p} \right)^{s/\omega} \right) \quad \text{and} \quad d(B) = \Omega \left( \left( \frac{n^\omega}{p} \right)^{t/\omega} \right),
\]
furthermore,
\[
W_\Psi(n, s, t, v, p) = \Omega \left( \left( \frac{n^\omega}{p} \right)^{\max(s,t)/\omega} \right).
\]
Identical arguments can be made for the cases when only \( s = 0 \) and only \( t = 0 \), yielding the formula in the theorem.

\[\square\]

9 Lower Bounds for the Symmetry Preserving Algorithm

We now derive communication cost lower bounds for the symmetry preserving algorithm. This algorithm performs less computation and has a lower rank than the direct evaluation algorithm we analyzed in the previous section. However, we determine that it has a different expansion bound and consequently different communication cost requirements. We again use Lemma 6.2 to prove the expansion bound for the symmetry preserving algorithm in order to lower bound the size of the projected sets (inputs and outputs of some algorithm subset). However, for the symmetry preserving algorithm, some of these projected sets can have a higher dimensionality than corresponding ones in the direct evaluation algorithm.

We show that both the vertical and horizontal communication cost lower bounds are asymptotically greater for the symmetry preserving algorithm than the direct evaluation algorithm, whenever \( 0 < \min(s, t, v) < \omega/3 \) (possible only when \( \omega \geq 4 \)). These cases correspond to matrix-matrix-like contractions, where the direct evaluation algorithm tensor unfoldings are nonsquare matrices.

**Lemma 9.1.** An expansion bound on \( \Phi_\omega^{(s,t,v)} \) is
\[
\mathcal{E}_{\Phi}^{(s,t,v)}(d(A), d(B), d(C)) = \min \left( \left( \left( \frac{\omega}{t} \right)^{d(A)} \right)^{\frac{s}{\omega}}, \left( \left( \frac{\omega}{s} \right)^{d(B)} \right)^{\frac{t}{\omega}}, \left( \left( \frac{\omega}{v} \right)^{d(C)} \right)^{\frac{1}{\omega}} \right).
\]

**Proof.** For \( \hat{\Lambda}_{s,t,v}^{(s,t,v)} = \Phi_\omega^{(s,t,v)} \), we have the following non-zero structure in the sparse tensors specifying the corresponding bilinear algorithm, \( \forall \bar{i} \in \mathbb{Z}[1, n]^\omega \),
\[
\forall (\bar{j}, \bar{a}) \in \hat{\chi}^{s+t+1}(\bar{i}), \quad K_{\bar{j} \bar{a}}^{(A)} = \frac{t!}{\rho(\bar{a})},
\]
\[
\forall (\bar{i}, \bar{b}) \in \hat{\chi}^{v+t+1}(\bar{i}), \quad K_{\bar{i} \bar{b}}^{(B)} = \frac{s!}{\rho(\bar{b})},
\]
\[
\forall (\bar{h}, \bar{c}) \in \hat{\chi}^{s+t+1}(\bar{i}), \quad K_{\bar{h} \bar{c}}^{(C)} = s! t! / \rho(\bar{c}).
\]

Consider any \( \Lambda^{(R)} \subseteq \hat{\Lambda}_{s,t,v}^{(s,t,v)} \) and the associated set of products, \( Z \subseteq D^{(M)} = \mathbb{Z}[1, n]^\omega \). We prove that \( d(A) := \text{rank}(R^{(A)}) \geq \lvert Z \rvert^{(s+v)/\omega}/\binom{n}{\omega} \). Let \( L^{(A)} \) be the number of rows in \( R^{(A)} \) that are nonzero,
\[
L^{(A)} = \{ \bar{j} : \bar{i} \in \hat{\chi}^{s+t+1}(\bar{i}), \bar{i} \in Z \}.
\]
Each column of \( R^{(A)} \) has at most \( \binom{n}{\omega} \) nonzeros. Therefore, since the columns of \( R^{(A)} \) to which set \( Z \) is mapped, contain nonzeros in \( L^{(A)} \) different rows, there exists a subset of these columns of size \( |L^{(A)}|/\binom{n}{\omega} \) where each column has a unique nonzero row, and consequently these columns are linearly-independent. Such a subset can be found
by successively picking columns with a nonzero row index that is not yet in the working set, and adding at most \(^\binom{\omega}{2}\) new indices to the working set with each added column. The existence of this subset of columns implies that 
\[
\text{rank}(R^{(A)}) \geq |L^{(A)}|.
\]

By Lemma 6.2, \(|L^{(A)}| \geq |Z|^{(s+v)}/\omega\) and so \(\text{rank}(R^{(A)}) \geq |Z|^{(s+v)}/\omega\). Identical arguments may be used to show the symmetric bounds \(d^{(B)} := \text{rank}(R^{(B)}) \geq |Z|^{(v+t)}/\omega\) and \(d^{(C)} := \text{rank}(R^{(C)}) \geq |Z|^{(s+t)}/\omega\). Combining the three bounds yields the bound in the lemma.

\[\square\]

### 9.1 Vertical Communication Lower Bounds for the Symmetry Preserving Algorithm

As done previously, we use the expansion bound to prove a lower bound on the vertical communication cost on the symmetry preserving algorithm. A previous proof of these communication lower bound on algorithm \(\Phi^{(s,t,v)}_\circ(A, B)\) appeared in [20]. It employed the lower bound technique from [7], which relies on the Hölder inequality [11] and its generalization [5]. The proof we provide here is more general as it allows for reuse of partial summations in computing operands of different products.

**Theorem 9.2.** Let \(\kappa := \max(s + v, v + t, s + t)\). Any schedule of \(\Phi^{(s,t,v)}_\circ\) on \(\mathcal{M}(H)\) has vertical communication cost,

\[
Q_\Phi(n, s, t, v, H) \geq \max \left[ \frac{2 \left(\binom{\omega}{3}\right) H}{(3^\kappa H)^{\omega/\kappa}}, \left( \binom{n}{s + v + t} \right) + \left( \binom{n}{v + t} \right) + \left( \binom{n}{s + t} \right) \right]
\]

\[= \Omega \left( \frac{n^\omega}{H^{\omega/\kappa - 1}} + n^\kappa \right) .
\]

**Proof.** Applying Theorem 5.2, with the expansion bound \(E^{(s,t,v)}_\Phi\), we obtain the vertical communication lower bound,

\[
Q_\Phi(n, s, t, v, H) \geq \max \left[ \frac{2 \left(\binom{\omega}{3}\right) H}{E^{(s,t,v)}_\Phi(H)} \left( \binom{n}{s + v} \right) + \left( \binom{n}{v + t} \right) + \left( \binom{n}{s + t} \right) \right] ,
\]

where

\[
E^{\max}_{\Phi}(H) := \max_{c(A), c(B), c(C) \in \mathbb{N}, c(A) + c(B) + c(C) = 3H} E_\Phi(c^{(A)}, c^{(B)}, c^{(C)}).
\]

Substituting \(E^{(s,t,v)}_\Phi\) from Lemma 9.1, we obtain,

\[
E^{\max}_{\Phi}(H) \leq E^{(s,t,v)}_\Phi(3H, 3H, 3H) = \left( \binom{\omega}{\kappa} H \right)^{\omega/\kappa} ,
\]

where \((\kappa := \max(s + v, v + t, s + t))\). Inserting this upper bound on \(E^{\max}_{\Phi}(H)\) into the cost lower bound on \(Q_\Phi(n, s, t, v, H)\), yields the cost lower bound shown in the theorem. \[\square\]

We note that this vertical commutation lower bound is asymptotically the same as that of the direct evaluation algorithm (Theorem 8.3) when \(\kappa = 2\omega/3\), or when one of \(s, t, v\) is zero. When \(s, t, v > 0\) and \(\kappa > 2\omega/3\) (so \(0 < \min(s, t, v) < \omega/3\)), this communication cost lower bound is asymptotically greater than that of Theorem 8.3.

### 9.2 Horizontal Communication Lower Bounds for the Symmetry Preserving Algorithm

We now derive a horizontal communication lower bound for parallel executions of the symmetry preserving algorithm. Again the lower bound is obtained directly by substitution of the expansion bound into Lemma 5.3 for general bilinear algorithms. The second horizontal communication lower bound for the direct evaluation algorithm (Theorem 8.5) is the same as the bound we prove below for the symmetry preserving algorithm when exactly one of \(s, t, v\) is zero. Like the vertical communication lower bound, the horizontal communication lower bound is greater for the symmetry preserving algorithm than for the direct evaluation algorithm, when \(0 < \min(s, t, v) < \omega/3\).

**Theorem 9.3.** Any storage-balanced schedule of \(\Phi^{(s,t,v)}_\circ(A, B)\) on \(\mathcal{M}(p)\) has horizontal communication cost,

1. \(W_\Phi(n, s, t, v, p) = \Omega \left( \frac{n^\omega}{p^{\kappa/\omega}} \right)\) with \(\kappa := \max(s + v, v + t, s + t)\), when \(s, t, v \geq 1\).
2. \( W_\varphi(n, s, t, v, p) = \Omega \left( \left( \frac{n^\omega}{p} \right)^{\max(s, t, v)/\omega} \right), \) when exactly one of \( s, t, v \) is zero.

**Proof.** By Lemma 9.1, we have the expansion bound,
\[
\mathcal{E}_{\Phi}^{(s, t, v)}(d(A), d(B), d(C)) = \min \left[ \left( \left( \frac{\omega}{t} \right)^{d(A)} \right)^{\frac{\omega}{s^v + 1}}, \left( \left( \frac{\omega}{s} \right)^{d(B)} \right)^{\frac{\omega}{v^t + 1}}, \left( \left( \frac{\omega}{v} \right)^{d(C)} \right)^{\frac{\omega}{s^t + 1}} \right].
\]

Applying Theorem 5.3, with expansion bound \( \mathcal{E}_{\Phi}^{(s, t, v)} \), we obtain the horizontal communication cost bound,
\[
W_\varphi(n, s, t, v, p) \geq d(A) + d(B) + d(C),
\]
with the constraint that \( d(A), d(B), d(C) \in \mathbb{N} \) and
\[
\left\lceil \frac{n}{p} \right\rceil \leq \mathcal{E}_{\Phi}^{(s, t, v)} \left( d(A) + \left( \frac{n}{s + v} \right)/p, d(B) + \left( \frac{n}{s + v} \right)/p, d(C) + \left( \frac{n}{s + v} \right)/p \right)
\]
\[
= \min \left[ \left( \left( \frac{\omega}{t} \right)^{d(A) + \left( \frac{n}{s + v} \right)/p} \right)^{\frac{\omega}{s^v + 1}}, \left( \left( \frac{\omega}{s} \right)^{d(B) + \left( \frac{n}{s + v} \right)/p} \right)^{\frac{\omega}{v^t + 1}}, \left( \left( \frac{\omega}{v} \right)^{d(C) + \left( \frac{n}{s + v} \right)/p} \right)^{\frac{\omega}{s^t + 1}} \right].
\]

When \( s, t, v \geq 1 \), this constraint implies that we must have
\[
\min \left( \left( d(A) \right)^{\frac{\omega}{s^v + 1}}, \left( d(B) \right)^{\frac{\omega}{v^t + 1}}, \left( d(C) \right)^{\frac{\omega}{s^t + 1}} \right) = \Omega \left( \left( \frac{n^\omega}{p} \right)/p \right).
\]
Furthermore, in this case, for \( \kappa = \max(s + v, v + t, s + t) \),
\[
W_\varphi(n, s, t, v, p) = \Omega \left( \left( \frac{n^\omega}{p} \right)^{\kappa/\omega} \right).
\]
However, when \( v = 0 \), \( \left( \frac{\omega}{v} \left( \frac{n}{s + t} \right)/p \right)^{\frac{\omega}{s^t + 1}} = \left\lceil \frac{n}{p} \right\rceil \), so we have only the constraint,
\[
\min \left( (d(A))^{\frac{\omega}{s^t + 1}}, (d(B))^{\frac{\omega}{s^t + 1}} \right) = \Omega \left( \left( \frac{n}{p} \right)/p \right).
\]
This constraint implies the lower bound,
\[
W_\varphi(n, s, t, 0, p) = \Omega \left( \left( \frac{n^\omega}{p} \right)^{\max(s, t)/\omega} \right).
\]
Similar arguments apply when instead of \( v = 0 \), we have \( s = 0 \) or \( t = 0 \). Combining the bounds from these three cases yields the general bound stated in the theorem. \( \square \)

## 10 Conclusion

We summarize the communication lower bound results obtained for different tensor contraction algorithms in Table 10.1. The first three columns \( (s, t, v) \) give the order of the tensor contraction operands: \( s + v \) and \( v + t \), as well as of the result, \( s + t \). The dimension (range of indices) of all modes of the tensors is given by \( n \). The following three columns \( (F_\varphi, F_\psi, F_\theta) \) provide the number of multiplications (to leading order in \( n \)) needed for nonsymmetric contractions, the direct evaluation algorithm for symmetric contractions, and the symmetry preserving algorithm, respectively. The last five columns in Table 10.1, list the asymptotic communication cost lower bounds (with \( \Omega \) omitted), where \( Q \) is vertical communication (\( H \) is the cache size) and \( W \) is horizontal communication. The vertical communication cost lower bounds for the nonsymmetric case and the direct evaluation algorithm are listed within one column, because the pair are always asymptotically equivalent. The table presents the lower bounds in simplified form with the use of the assumptions: \( n \geq p \gg 1 \) and \( H \leq n^2 \). These assumptions are sensible when \( \omega = s + t + v \) is small.
Table 10.1: The table presents bilinear rank ($F$) and communication cost lower bounds ($Q$—vertical and $W$—horizontal) for nonsymmetric and symmetric tensor contraction algorithms ($\Upsilon$—nonsymmetric, $\Psi$—direct evaluation, $\Phi$—symmetry preserving). Row 2 gives the general costs for matrix-vector-like contractions, and rows 3-6 list particular instances. Row 7 gives the general cost for matrix-matrix-like contractions, and rows 8-11 list particular instances. The results are symmetric in permutation of $(s, t, v)$, so we focus on $s \geq t \geq v$. Green coloring shows where improvements obtained via symmetry, while red coloring identifies overheads of exploiting it.

| s | t | v | $F_\Upsilon$ | $F_\Psi$ | $F_\Phi$ | $Q_{\Upsilon, \Psi}$ | $Q_\Phi$ | $W_{\Upsilon}$ | $W_\Psi$ | $W_\Phi$ |
|---|---|---|---|---|---|---|---|---|---|---|
| $\geq t$ | $\geq 1$ | 0 | $n^s \omega$ | $n^s \omega$ | $n^s \omega$ | $n^s \omega$ | $\min\left(n^t, \frac{n^s}{p^3/\tau}\right)$ | $\frac{n^s}{p^3/\tau}$ | $\frac{n^s}{p^3/\tau}$ |
| 1 | 1 | 0 | $n^4$ | $\frac{n^4}{2}$ | $n^3$ | $n^2$ | $n^2$ | $\frac{n}{p^{1/2}}$ | $\frac{n}{p^{1/2}}$ | $\frac{n}{p^{1/2}}$ |
| 2 | 1 | 0 | $n^3$ | $\frac{n^3}{2}$ | $n^2$ | $n^2$ | $\frac{n^2}{p^{1/2}}$ | $\frac{n^2}{p^{1/2}}$ | $\frac{n^2}{p^{1/2}}$ |
| 3 | 1 | 0 | $n^3$ | $\frac{n^3}{2}$ | $n^2$ | $n^2$ | $\frac{n^2}{p^{1/2}}$ | $\frac{n^2}{p^{1/2}}$ | $\frac{n^2}{p^{1/2}}$ |
| 2 | 2 | 0 | $n^4$ | $\frac{n^4}{2}$ | $n^3$ | $n^3$ | $\frac{n^3}{p^{1/2}}$ | $\frac{n^3}{p^{1/2}}$ | $\frac{n^3}{p^{1/2}}$ |

To draw conclusions from lower bounds, it is important to also consider their attainability. The matrix multiplication and nonsymmetric tensor contraction vertical communication lower bounds are easily attainable by reading in $\sqrt{H/3} \times \sqrt{H/3}$ blocks of each matrix. The parallel horizontal communication bounds for these nonsymmetric algorithms are also attainable for all dimensions [10].

The vertical communication lower bounds for the direct evaluation algorithm, $\Psi_{s,t,v}^o(A, B)$, are asymptotically attainable by use of an efficient matrix multiplication algorithm, however, attaining the constant factors is more difficult. When one of $s, t, v$ is zero, they may be attained by exploiting the symmetry of the largest tensor for each block loaded in cache.

The parallel horizontal communication lower bounds for the direct evaluation algorithm should be asymptotically attainable when $s, t, v > 0$ by unpacking the tensors and performing an efficient matrix multiplication algorithm [18, 23]. When exactly one of $s, t, v$ is zero, storing the largest tensor in packed layout and moving the other operands should asymptotically attain the lower bounds presented in this paper. It is also interesting to ask whether it is sometimes worth storing tensors in unpacked layout when the memory is available, as this permits lower communication cost for some matrix-vector-like contractions.

For the symmetry preserving algorithm, $\Phi_{s,t,v}^o(A, B)$, the sequential vertical communication cost can be attained within a constant factor by the algorithm given in [20]. We conjecture that the parallel bounds may also be attained asymptotically for any choice of $(s, t, v)$.

Our lower bounds demonstrate that the symmetry preserving algorithm has the same asymptotic communication bounds as the direct evaluation algorithm for the types of (anti)symmetry in coupled cluster contractions (always matrix-vector-like). However, coupled-cluster contractions generally involve partially symmetric tensors, which can be efficiently computed via nested use of the symmetry preserving algorithm [22]. These algorithms for partially-symmetric contractions are themselves still bilinear algorithms and, moreover, they can be derived via tensor (Kronecker) products as $\Lambda^{(F)} = \Lambda^{(G)} \otimes \Lambda^{(H)}$, where $F^{(A)} = G^{(A)} \otimes H^{(A)}$, $F^{(B)} = G^{(B)} \otimes H^{(B)}$, and $F^{(C)} = G^{(C)} \otimes H^{(C)}$. However, the systematic extension of the bilinear algorithm expansion bounds for nested bilinear algorithms is non-trivial, so we leave it for future work.

Overall, our analysis provides an important step towards full characterization of the communication costs necessary.
for contractions of tensors with all possible types of permutational index symmetry. Tight bounds on the communication cost of such contractions would provide communication cost bounds for tensor-contraction-based methods such as coupled-cluster. Further, the infrastructure we develop for bilinear algorithms is extensible not only to partially-symmetric tensors, but also to contractions of sparse or structured tensors (e.g. Toeplitz or Henkel matrices). Our notion of expansion bounds for bilinear algorithms provides a unified way of quantifying the communication costs of all such tensor computations.

References

[1] Albert Alexandrov, Mihai F. Ionescu, Klaus E. Schauser, and Chris Scheiman. LogGP: incorporating long messages into the LogP model – one step closer towards a realistic model for parallel computation. In Proceedings of the Seventh Annual ACM Symposium on Parallel Algorithms and Architectures, SPAA ’95, pages 95–105, New York, NY, USA, 1995. ACM.

[2] Grey Ballard, James Demmel, Olga Holtz, and Oded Schwartz. Minimizing communication in linear algebra. *SIAM J. Mat. Anal. Appl.*, 32(3), 2011.

[3] Grey Ballard, James Demmel, Olga Holtz, and Oded Schwartz. Graph expansion and communication costs of fast matrix multiplication. *J. ACM*, 59(6):32:1–32:23, January 2013.

[4] Rodney J Bartlett. Many-body perturbation theory and coupled cluster theory for electron correlation in molecules. 32(1):359–401, 1981.

[5] Jonathan Bennett, Anthony Carbery, Michael Christ, and Terence Tao. The Brascamp–Lieb inequalities: finiteness, structure and extremals. *Geometric and Functional Analysis*, 17(5):1343–1415, 2008.

[6] Gianfranco Bilardi and Lorenzo De Stefani. The I/O complexity of Strassen’s matrix multiplication with recomputation. *arXiv preprint arXiv:1605.02224*, 2016.

[7] Michael Christ, James Demmel, Nicholas Knight, Thomas Scanlon, and Katherine Yelick. Communication lower bounds and optimal algorithms for programs that reference arrays–part 1. *arXiv preprint arXiv:1308.0068*, 2013.

[8] Pierre Comon, Gene Golub, Lek-Heng Lim, and Bernard Mourrain. Symmetric tensors and symmetric tensor rank. *SIAM Journal on Matrix Analysis and Applications*, 30(3):1254–1279, 2008.

[9] David Culler, Richard Karp, David Patterson, Abhijit Sahay, Klaus Erik Schauser, Eunice Santos, Ramesh Subramonian, and Thorsten von Eicken. LogP: towards a realistic model of parallel computation. In *Proceedings of the Fourth ACM SIGPLAN Symposium on Principles and Practice of Parallel Programming*, PPOPP ’93, pages 1–12, New York, NY, USA, 1993. ACM.

[10] James Demmel, David Eliahu, Armando Fox, Shoaiib Kamil, Benjamin Liphsitz, Oded Schwartz, and Omer Spillinger. Communication-optimal parallel recursive rectangular matrix multiplication. In *IEEE International Symposium on Parallel Distributed Processing (IPDPS)*, 2013.

[11] Otto Hölder. Über einen Mittelwertsatz. *Nachrichten von der König. Gesellschaft der Wissenschaften und der Georg-Augusts-Universität zu Göttingen*, pages 38–47, 1889.

[12] Hong Jia-Wei and H. T. Kung. I/O complexity: The red-blue pebble game. In *Proceedings of the thirteenth annual ACM Symposium on Theory of Computing*, STOC ’81, pages 326–333, New York, NY, USA, 1981. ACM.

[13] Tamara G Kolda and Brett W Bader. Tensor decompositions and applications. *SIAM Review*, 51(3):455–500, 2009.

[14] Chuck L. Lawson, Richard J. Hanson, David R Kincaid, and Fred T. Krogh. Basic Linear Algebra Subprograms for Fortran usage. *ACM Transactions on Mathematical Software (TOMS)*, 5(3):308–323, 1979.

[15] Lynn H. Loomis and Hassler Whitney. An inequality related to the isoperimetric inequality. *Bulletin of the AMS*, 55:961–962, 1949.
[16] Jozef Noga and Pierre Valiron. Improved algorithm for triple-excitation contributions within the coupled cluster approach. *Molecular Physics*, 103(15-16):2123–2130, 2005.

[17] Victor Pan. How can we speed up matrix multiplication? *SIAM review*, 26(3):393–415, 1984.

[18] Samyam Rajbhandari, Akshay Nikam, Pai-Wei Lai, Kevin Stock, Sriram Krishnamoorthy, and P. Sadayappan. A communication-optimal framework for contracting distributed tensors. In *Proceedings of the International Conference for High Performance Computing, Networking, Storage and Analysis, SC ’14*, pages 375–386, Piscataway, NJ, USA, 2014. IEEE Press.

[19] Jacob N Scott. *An I/O-Complexity Lower Bound for All Recursive Matrix Multiplication Algorithms by Path-Routing*. PhD thesis, UNIVERSITY OF CALIFORNIA, BERKELEY, 2015.

[20] Edgar Solomonik. *Provably efficient algorithms for numerical tensor algebra*. PhD thesis, University of California, Berkeley, 2014.

[21] Edgar Solomonik, Erin Carson, Nicholas Knight, and James Demmel. *Tradeoffs between synchronization, communication, and computation in parallel linear algebra computations*, pages 307–318. *SPAA ’14*. ACM, New York, NY, USA, 2014.

[22] Edgar Solomonik and James Demmel. Contracting symmetric tensors using fewer multiplications. Technical report, ETH Zurich, 2015.

[23] Edgar Solomonik, Devin Matthews, Jeff R. Hammond, John F. Stanton, and James Demmel. A massively parallel tensor contraction framework for coupled-cluster computations. *Journal of Parallel and Distributed Computing*, 74(12):3176 – 3190, 2014.

[24] Volker Strassen. Gaussian elimination is not optimal. *Numerische Mathematik*, 13(4):354–356, 1969.

[25] Alexander Tiskin. *The design and analysis of bulk-synchronous parallel algorithms*. PhD thesis, University of Oxford, 1998.

[26] Leslie G. Valiant. A bridging model for parallel computation. *Communications of the ACM*, 33(8):103–111, 1990.

[27] Jiří Čížek. On the correlation problem in atomic and molecular systems. calculation of wavefunction components in ursell-type expansion using quantum-field theoretical methods. *The Journal of Chemical Physics*, 45(11):4256–4266, 1966.