# Matrix Multiplication I/O-Complexity by Path Routing

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# ABSTRACT

We apply a novel technique based on path routings to obtain optimal I/O-complexity lower bounds for all Strassenlike fast matrix multiplication algorithms computed in serial or in parallel, assuming no reuse of nontrivial intermediate linear combinations. Given fast memory of size M, we prove an I/O-complexity lower bound of  $\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\omega_0}, M\right)$ for any Strassen-like matrix multiplication algorithm applied to  $n \times n$  matrices of arithmetic complexity  $\Theta(n^{\omega_0})$  with  $\omega_0 < 3$  under this assumption. This generalizes an approach by Ballard, Demmel, Holtz, and Schwartz that provides a tight lower bound for Strassen's matrix multiplication algorithm but which does not apply to algorithms with disconnected encoding or decoding components of the underlying computation graph or algorithms with multiply copied values. We overcome these challenges via a new graphtheoretical approach for proving I/O-complexity lower bounds without the use of edge expansions.

## **Categories and Subject Descriptors**

F.2.1 [Analysis of Algorithms and Problem Complexity]: Numerical Algorithms and Problems; Computations on matrices

## **General Terms**

Algorithms, Design, Performance

## **Keywords**

Communication-avoiding algorithms; Fast matrix multiplication; I/O-complexity

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# 1. INTRODUCTION

In practice, most of the runtime of an algorithm is often due to the communication of data within memory hierarchy and between multiple processors, rather than the arithmetic computations. The amount of communication performed during an algorithm depends on the order in which intermediate values are computed and kept in/discarded from cache. While much work has gone into constructing implementations of algorithms that reduce communication, in this paper we show lower bounds on the communication of any implementation of a common class of fast (but not classical; see Lemma 1) matrix multiplication algorithms.

The I/O-complexity of an algorithm is defined as the minimum possible number of cache operations required to compute all outputs of the algorithm using a fixed cache size M. In 2011, Ballard, Demmel, Holtz, and Schwartz showed a tight lower bound on the I/O-complexity of Strassen's fast matrix multiplication algorithm [6]. We prove an analogous I/O-complexity bound via a more general technique for any fast square matrix multiplication algorithm based on a uniform recursive step that does not recompute any intermediate values, subject to the assumption that every intermediate linear combination is used in only one multiplication. We also claim, without proof, that this assumption can be lifted. Because algorithms achieving our I/O-complexity bounds have been found [3], our bounds are optimal.

#### Machine model

In this paper, we assume a 2-layer memory hierarchy for sequential computations consisting of slow memory and fast memory. The slow memory is of unlimited size and represents the hard drive of a computer, while the fast memory, called cache, is of limited size M and may represent RAM. We model the I/O communication of an algorithm as follows: initially, all data resides in slow memory and the cache is empty. A single value may be input into cache from slow memory or output to slow memory from cache for the cost of one I/O. A computation in the algorithm may only be performed if all input values to that computation already reside in cache; when computed, the result is also put in cache. The algorithm halts when all outputs of the algorithm are stored in slow memory. In this model we assume that no arithmetic computation is ever performed more than once. See [10] for the formalization of this model as a pebble game played on the computation graph.

The number of cache I/Os (henceforth simply called I/Os) required may depend on the order in which intermediate values of the algorithm are computed. The algorithm's I/O-

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*complexity* is thus defined as the minimum number of I/Os over all sequences of computations and I/Os that computes the algorithm's outputs.

For parallel computations we consider P processors, each having independent local memory of size M. As in [6] and [16], we define the bandwidth cost of an algorithm executed in parallel to be the number of values communicated between processors along the critical path. In other words, we count the total number of words (single values) sent between processors, except that words sent between processors simultaneously count as only one I/O. We call this the *bandwidth cost* of the algorithm.

### **Previous Work**

In 1981 Hong and Kung [10] proved a tight lower bound on the I/O-complexity of the classical  $\Theta(n^3)$  matrix multiplication algorithm (achieved by blocked multiplication) using S-partitions. A different proof of this result was given in [12] and later generalized in [5] via the Loomis-Whitney inequality [13]; this approach was also shown to apply to several other problems in numerical linear algebra. See [1] and [9] for further generalizations using other geometric bounds. However, these proofs apply only to direct numerical linear algebra algorithms, but not to algorithms that use distributivity for cancellation, such as Strassen's algorithm.

The edge expansion approach detailed in [6] relates the I/O-complexity of an algorithm to the edge expansion properties of the underlying computation graph. This technique provides an I/O-complexity lower bound for Strassen's fast matrix multiplication algorithm, but fails for algorithms with base graphs (the computation graph representing one recursive step; see Section 3) containing disconnected encoding or decoding graphs and those involving multiple copying. In [4], this approach is extended to fast recursive matrix multiplication algorithms for rectangular matrices whose base graphs consist of multiple equal-size connected components. This is sufficient to yield lower bounds for some common fast matrix multiplication algorithms, such as Bini's algorithm [8] and the Hopcroft-Kerr algorithm [11], but still does not address algorithms with general base graphs.

In this paper we present the first approach for proving I/O-complexity lower bounds for recursive fast matrix multiplication algorithms involving arbitrary base graphs, as long as the same base graph is used at each recursive step.

## 2. NEW APPROACH

Most previous lower bounds in this field are based on the Loomis-Whitney inequality (as in [12]), dominator sets/S-partitions (as in [10], [14], and [7]), or edge expansions (as in [6] and [4]). In this paper we apply a new technique, based on the existence of a routing of paths within the underlying computation graph. In particular, we show the existence of a set of paths between all the inputs and all the outputs of sufficiently large matrix multiplication subcomputations such that each vertex is hit relatively few times. We then show that if some, but not all, of these input and output vertices are to be computed in one computation segment, then there must exist many other vertices that contribute cache I/Os as a result. This new approach may generalize to other problems that have sufficient symmetry to guarantee the existence of an efficient routing.

## **3. PRELIMINARIES**

As in [6], we define the computation directed acyclic graph (CDAG) of an algorithm to be the directed graph that contains a vertex for every value in the computation (input, output, or intermediate value) and an edge whenever one value depends directly on another.

Strassen's matrix multiplication algorithm works as follows: to multiply  $2 \times 2$  matrices A and B, compute specific linear combinations of the entries of A and linear combinations of the entries of B, perform 7 multiplications of these linear combinations, and then take linear combinations of the results to get the entries of C = AB. For larger square input matrices, divide each input matrix in half horizontally and vertically and apply the above procedure, recursively computing the necessary products of submatrices.

A Strassen-like algorithm is a square matrix multiplication algorithm that takes a similar form: to multiply matrices of dimensions  $n_0 \times n_0$ , take linear combinations of the input matrices, compute products, and take linear combinations of the results to yield the entries of the output matrix. For larger matrices, divide into blocks and recurse.

Let  $G_r$  be the CDAG of a Strassen-like algorithm for  $n_0^r \times n_0^r$  square matrix multiplication C = AB, necessarily consisting of r recursive levels. We call  $G_1$  the base graph.  $G_1$  consists of two encoding graphs, which compute linear combinations of entries of A and of B, a multiplication layer with b multiplication vertices, which compute products of these linear combinations, and then a decoding graph, which takes linear combinations of these products to yield the entries of C. Note that  $G_1$  has  $2n_0^2$  inputs,  $n_0^2$  from each input matrix. Further note that the same linear combination of input elements may be used as inputs in multiple product vertices. In this paper all figures show computations that proceed from bottom to top; we therefore omit the directions of edges. See Figure 1.

Figure 1: The base graph  $G_1$  of Strassen's algorithm for multiplying two  $2 \times 2$  matrices A and B. Here b = 7.



Note that  $G_r$  is a ranked graph, with inputs on rank 0 and outputs on rank 2r. Ranks 0 through r lie in the encoding graphs and ranks r+1 through 2r lie in the decoding graph; the multiplication layer occurs between ranks r and r+1.

An intermediate vertex in  $G_r$  may have a single input vertex and, in this case, may have the same value as its one input. We call this *copying*; if the same value is copied to more than one child vertex, we call it *multiple copying*. We could consider this an artifact of our drawing of  $G_r$  and choose to identify these vertices. However, doing so would break the simple ranked, recursive structure of  $G_r$ . Instead, we group all vertices that represent the same value into a single *meta-vertex*. The vertices corresponding to each metavertex form a chain in the case of single copying and an upwards-branching subtree of the CDAG in the case of multiple copying, where each vertex of the subtree apart from the root has no other edges entering it from below. See Figure 2 for a depiction of a meta-vertex in the case of multiple copying. For most of this paper we consider only vertices, not meta-vertices, and then show that our technique still applies when copying or multiple copying occurs.

Figure 2: The meta-vertex corresponding to copies of the vertex v. Edges whose endpoints are not shown denote edges to vertices not in the shown meta-vertex. If this meta-vertex is in the CDAG for Strassen-like matrix multiplication, the structure of the meta-vertex is actually more regular than depicted due to the simple recursion.



The approach in [6] fails when the decoding graph of the base graph  $G_1$  has a disconnected encoding or decoding graph. Note that the entire CDAG  $G_r$  (and similarly  $G_1$ ) must be connected simply because it computes matrix multiplication (this will be shown in greater detail in the process of proving Lemma 4), but the decoding graph and/or encoding graph may not be connected individually.

In this paper, we first demonstrate a technique to derive the I/O-complexity bound for Strassen's algorithm presented in [6] more easily. We then show how to extend the technique, via use of Theorem 2, to the case of disconnected decoding and/or encoding graphs, allowing us to derive strong lower bounds for all Strassen-like matrix multiplication algorithms in which each linear combination is used in only one multiplication. This will prove Theorem 1, our main result. Finally, we present a proof of Theorem 2.

THEOREM 1 (MAIN THEOREM). Let a and b be small constants. Consider a Strassen-like matrix multiplication algorithm for  $n \times n$  matrices with arithmetic complexity  $o(n^3)$ using cache size  $M \leq o(n^2)$  in which the base graph has 2a inputs and b outputs. If in the base graph every nontrivial linear combination of elements of the input matrices is used in only one multiplication, then the algorithm has I/O-complexity

$$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{2\log_a b} \cdot M\right).$$

If run on P processors each of local cache size M, then the bandwidth cost is

$$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{2\log_a b} \cdot \frac{M}{P}\right).$$

In other words, if a Strassen-like matrix multiplication algorithm performs  $\Theta(n^{\omega_0})$  arithmetic operations with  $\omega_0 < 3$ , then its I/O-complexity is

$$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\omega_0}\cdot M\right).$$

If run on P processors, the bandwidth cost is

$$\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\omega_0}\cdot\frac{M}{P}\right).$$

Furthermore, regardless of the cache size the bandwidth cost is

$$\Omega\left(\frac{n^2}{P^{2/\omega_0}}\right)$$

as long as computation is load balanced per rank of the computation graph.

In [3] an explicit algorithm is given that attains the bounds in Theorem 1. The sequential-to-parallel argument from [2] (as well as [6], [12], and [5]) allows us to take P = 1 – that is, work entirely in the serial model – and get the factor of  $\frac{1}{P}$  in the parallel case with no additional work. Therefore, the remainder of this paper is devoted to proving a lower bound of  $\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{2\log_a b} \cdot M\right)$  in the sequential case, from which Theorem 1 follows. By [3], the lower bounds in Theorem 1 are optimal.

## 4. **DEFINITIONS**

The proof presented in [6] relies on the notion of edge expansion; it shows a lower bound for the edge expansion of small subsets of vertices of the CDAG for Strassen's algorithm and then applies a lemma to yield a better edge expansion bound that relies on the fact that  $G_r$  contains as subgraphs many edge-disjoint copies of  $G_k$  for k < r. In our proof we bypass edge expansions entirely by explicitly cutting  $G_r$  into many copies of  $G_k$  for k < r. Both methods rely on the following fact, which is a consequence of the recursive definition of Strassen-like algorithms:

FACT 1. For  $0 \le k \le r$ , let  $G_{r,k}$  be the induced subgraph of  $G_r$  formed by the middle 2(k+1) levels of vertices (i.e. ranks r - k through r of the encoding graphs and rank 0through k of the decoding graph). Then  $G_{r,k}$  consists of  $b^{r-k}$ vertex-disjoint copies of the graph  $G_k$ .

In other words, the middle 2(k+1) layers of  $G_r$  are responsible for computing  $b^{r-k}$  independent matrix multiplications of square matrices of size  $n_0^k \times n_0^k$ .

DEFINITION 1. For any subset S of vertices of a computation graph G with directed edges E, define the following:

- 1.  $R(S) = \{v \in G S \mid \text{ for some } w \in S, (v, w) \in E\}$
- 2.  $W(S) = \{v \in S \mid \text{ for some } w \in G S, (v, w) \in E\}$

3. 
$$\delta(S) = R(S) \bigcup W(S)$$

Note that R(S) and W(S) are disjoint, so  $|\delta(S)| = |R(S)| + |W(S)|$ . If S denotes a set of consecutively-computed vertices of G, then R(S) denotes the set of vertices of G that must be read into cache, if not already present, during the computation of the vertices of S, and W(S) the set of vertices of G that must be written to cache, if not to remain in cache after the computation of S. We assume that no vertex in G is ever computed more than once, meaning that if a vertex is used in the computations of multiple other vertices, it must either remain in cache until all the computations of vertices depending on it have finished or else be written to and read from cache.

We also assume that every linear combination of inputs in the base graph – except for the inputs themselves – is used in at most one multiplication in the base graph; this implies that every meta-vertex in the base graph is either a single vertex or else is rooted at one of the input vertices.

If S' is a subset of meta-vertices of G, we similarly define  $\delta'(S') = \{ \text{meta-vertex } v' \text{ of } G \text{ not in } S' \mid$ for some  $w' \in S', v' \text{ and } w' \text{ are adjacent} \},$ 

where two meta-vertices v' and w' are considered to be adjacent}, cent if for some vertex  $v \in v'$  and vertex  $w \in w'$ ,  $(v, w) \in E$ or  $(w, v) \in E$ . In other words,  $\delta'(S')$  is the set of metavertices adjacent to any of those in S'.

The main proof in this paper is based on finding routings of paths between sets of vertices in subgraphs of the CDAG that avoid using any vertex too many times. To this end we make the following definition:

DEFINITION 2. If X and Y are subsets of the vertices V(G) of a directed graph G, define an m-routing between X and Y to be a collection R of |X||Y| paths such that for any  $x \in X$  and  $y \in Y$  there exists a path, ignoring the directedness of edges, in G between x and y and such that every vertex of G is used collectively amongst all the paths in R at most m times. Similarly, if F is a subset of  $V(G) \times V(G)$ , define an m-routing for F to be a collection of paths, one for every  $(v, w) \in F$ , such that every vertex of G is hit at most m times.

We will consider only the case where X and Y are disjoint. Note that *m*-routings need not be unique, and in fact part of the challenge of our proof is constructing a canonical *m*routing with sufficiently small *m*.

DEFINITION 3. Let G = (V, E) and  $S \subseteq V$ . If p is a path in G that contains at least one vertex in S and at least one vertex in G - S, then we call p boundary-crossing with respect to S in G.

Note that any boundary-crossing path contains a pair of adjacent vertices such that one is in S and the other is not. Our basic strategy will be to show the existence of *m*-routings for relatively small m, and then show that such a routing must contain many boundary-crossing paths, implying the existence of many vertices in  $\delta(S)$  and thus many meta-vertices in  $\delta'(S')$ .

# 5. SIMPLE PROOF FOR STRASSEN'S AL-GORITHM

First we use our technique to rederive the lower bound on the I/O-complexity for Strassen's algorithm presented in [6],  $\Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{\log_2 7} \cdot M\right)$ . As in [6], we consider the sequence of computations of vertices performed by the algorithm. In [6], this sequence is divided up into segments of sufficient length such that the I/O due to each segment is guaranteed to be at least M, the cache size. To do this, the smallest segment length s is found such that for any segment S of size s we are guaranteed that  $|\delta(S)| \geq 3M$ . All vertices present in  $\delta(S)$  contribute to the I/Os due to S, except for vertices in R(S) already present in cache (at most M) and vertices in W(S) that need not be written to cache (at most M). Because [6] considers only the decoding graph of  $G_r$ , there are no concerns about vertex copying.

We use the same basic argument, but instead divide the sequence of vertex computations of the CDAG  $G_r$  into the smallest segments possible such that each segment S (except perhaps the last segment) contains 66M vertices from rank k of the decoding graph (rank r + k of  $G_r$ )<sup>1</sup>. When a vertex v is in S we consider every vertex in the same meta-vertex as v to also be in S; however, because there is no copying in the decoding graph every meta-vertex can contain only one vertex from the decoding graph. Note that the size of each segment may be different; we care only about the number of vertices on this specific rank. We let  $k = \lceil \log_4(132M) \rceil$ , the smallest integer k such that  $4^k \ge 2 \cdot 66M$ . Because rank k of the decoding graph contains  $4^k 7^{r-k}$  vertices, there are  $\lfloor \frac{4^k 7^{r-k}}{66M} \rfloor$  such complete segments. Let S be one such complete segment and let  $\bar{S}$  denote the vertices in S on rank k of the decoding graph of  $G_r$ . Thus we pick S as small as possible such that  $|\bar{S}| = 66M$ . If  $G_r$  is the CDAG for Strassen's algorithm for multiplying  $n_0^r \times n_0^r$  matrices, recall that  $G_{r,k}$  contains  $7^{r-k}$  copies of the graph  $G_k$ . For  $1 \leq i \leq j$  $7^{r-k}$ , let  $G_k^i$  be the *i*th such copy,  $S_i$  be the subset of S in  $G_k^i$ , and  $\bar{S}_i$  be the subset of vertices of  $S_i$  on rank k of  $G_r$ .

Intuitively, we "count" S by the number of vertices of S on this particular rank. It is these vertices that will contribute, perhaps indirectly, to I/Os performed during the computation of S, regardless of what vertices on other ranks lie in S.

Let  $D_k$  be the decoding graph of  $G_k$ . We now claim that there exists a routing of paths between all the input vertices and output vertices of  $D_k$  such that no vertex of  $D_k$  is hit too often:

CLAIM 1. There exists an  $(11 \cdot 7^k)$ -routing in  $D_k$  between the set of inputs of  $D_k$  and the set of outputs of  $D_k$ .

PROOF. If  $D_1$  were simply the complete graph  $K_{7,4}$ , there would exist a very natural routing of paths between inputs and outputs of  $D_k$ : for any input and output, there is a unique chain of vertices between them defined by the sequence of subcomputations the input lies in. A vertex on rank *i* of  $D_k$  is then hit  $7^i 4^{k-i} \leq 7^k$  times in this routing, once for every pair of input vertex beneath it and output vertex above it.

Unfortunately,  $D_1$  is not a complete graph. However, because  $D_1$  is connected there still exists a path within each copy of  $D_1$  from any input vertex to any output vertex.

 $<sup>^1\</sup>mathrm{We}$  did not optimize for the constant factor.

Where each path previously went directly from an input vertex v to an output vertex w of each  $D_1$ , it will now take any path (that doesn't repeat vertices) through the same  $D_1$  component from v to w. This idea is depicted in Figure 3. This multiplies the number of times a vertex is hit in the routing by at most the number of vertices in  $D_1$ , 11.  $\Box$ 

Figure 3: One of the encoding graphs in  $G_1$  for Strassen's algorithm. Because there is no edge from v to w, a chain must instead take a more indirect path, shown in red, through the encoding graph.



Each  $G_k^i$  contains a copy of  $D_k$  – for this proof we consider only the decoding piece  $D_k$  of  $G_k$ , but in the full proof we must consider  $G_k$  in its entirety in order to account for base graphs with disconnected encoding/decoding portions. Let  $D_k^i$  be the copy of  $D_k$  lying in  $G_k^i$  and note that  $|\bar{S}_i| \leq \frac{1}{2}4^k$ , so at most half of the vertices on the top rank of  $D_k^i$  are in S. For each  $1 \leq i \leq 7^{r-k}$ , fix an  $(11 \cdot 7^k)$ -routing in  $D_k^i$ between the  $7^k$  inputs and  $4^k$  outputs. See Figure 4. There are now two cases:

- 1. Fewer than half of the  $7^k$  vertices on the bottom rank of  $D_k^i$  are in S. In this case, there exist at least  $|\bar{S}_i| \frac{1}{2} 7^k$ paths in the routing going from an input to  $D_k^i$  not in S to an output in S.
- 2. At least half of the vertices on the bottom rank of  $D_k^i$  are in S. In this case, there exist at least  $(4^k |\bar{S}_i|) \frac{1}{2}7^k$  paths in the routing going from an input in S to an output not in S.

In either case, there are at least  $\frac{1}{2}|\bar{S}_i|7^k$  boundary-crossing (between  $S_i$  and  $D_k^i - S_i$ ) paths in the routing. Associate to each boundary-crossing path an edge in the path that crosses between  $S_i$  and  $D_k^i - S_i$ . The vertex of this edge that is not in S lies in  $\delta(S_i)$ . By the definition of *m*-routing,

$$|\delta(S_i)| \ge \frac{\frac{1}{2}|\bar{S}_i|7^k}{11 \cdot 7^k} = \frac{1}{22}|\bar{S}_i|$$

Adding this up over all the  $\bar{S}_i$  yields

$$|\delta(S)| \ge \sum_{i=1}^{7^{r-\kappa}} \frac{1}{22} |\bar{S}_i| = \frac{1}{22} |\bar{S}| \tag{1}$$

This step relies on the  $D_k$  being disjoint and the lack of copying in the decoding graph of Strassen's (or any Strassenlike) matrix multiplication algorithm. If multiple copying did occur, vertices in the different  $D_k^i$  need not correspond to distinct computations. This will add an additional layer of complexity to the upcoming proof. Since  $|\bar{S}|$  was chosen to be 66*M*, this yields  $\delta(S) \geq 3M$ . Therefore the computation of *S* contributes at least *M* I/Os. Thus the total I/O is at least

$$\left\lfloor \frac{4^{k}7^{r-k}}{66M} \right\rfloor \cdot M = \Omega\left(7^{r}\left(\frac{4}{7}\right)^{k}\right) = \Omega\left(|V(G_{r})|\frac{M}{M^{\log_{4}7}}\right)$$
$$= \Omega\left(\left(\frac{n_{0}}{\sqrt{M}}\right)^{\log_{2}7} \cdot M\right)$$

as long as  $M \leq o(n_0^2)$  (which guarantees that  $66M \leq 4^k 7^{r-k}$ ).  $\Box$ 

Figure 4: An example of a path considered in the  $(11 \cdot 7^k)$ -routing between an input vertex (to  $D_k^1$ ) that is not in S and an output vertex that is in S. The submultiplications are shown in red,  $S_1$  is shown in blue, and  $\overline{S}_1$  is circled. Note that the path zags up and down, as explained in Figure 3. For simplicity, only one encoding graph is shown and only 3 submultiplications are drawn.



#### 6. STRASSEN-LIKE ALGORITHMS

We now turn our attention to Strassen-like square matrix multiplication algorithms. Several nuances prevent our above proof from working as-is:

- 1.  $G_1$  may have disconnected encoding or decoding graphs. This prevents us from finding an *m*-routing in the decoding graph  $D_k$  because  $D_k$  itself may no longer be connected. We will solve this problem by considering  $G_k$ , consisting of the decoding graph as well as the two encoding graphs. The paths in our *m*-routing will no longer be chains or even chains with length 1 "zags," but may need to bounce between inputs and outputs of  $G_k$  several times. See Figure 5.
- 2. Multiple copying may occur in the encoding graphs. This means a collection of *m*-routings for the  $G_k^i$  could potentially hit a meta-vertex more than *m* times. We will show via Theorem 2 that *m*-routings will only hit a meta-vertex entirely within  $G_k$  at most *m* times and then change the overall counting argument slightly to prevent meta-vertices between multiple  $G_k^i$ s from being hit too often.

As before, we divide the sequence of vertex computations of  $G_r$  into segments such that each segment S contains enough vertices of a certain type. Again let  $G_k^i$  be the *i*th subcomputation of  $G_{r,k}$  for  $1 \leq i \leq b^{r-k}$ . Let a *duplicated* vertex be a vertex of the CDAG  $G_r$  with at least one other copy (called a *duplicate*) in  $G_r$ , that is one whose meta-vertex contains more than one vertex. We call two subcomputations *input-disjoint* if none of their inputs lie in the same meta-vertex.

Let S be a segment of the sequence of vertex computations. Recall that when  $v \in S$  we consider every vertex w in the same meta-vertex as v to also be in S. For this argument we count only the vertices on rank k of the decoding graph of  $G_r$  and rank r - k of either encoding graph that are in mutually input-disjoint subcomputations  $G_{r,k}$ . We choose  $k = \lceil \log_a 72M \rceil$ , the smallest integer k such that  $a^k \geq 2 \cdot 36M$ .

First we show that counting only vertices lying in subcomputations that do not share inputs reduces the number of vertices on the relevant ranks by only a constant factor.

LEMMA 1. Let  $k \leq r-2$ . If not every vertex in the encoding graph for A of  $G_1$  is a duplicated vertex and similarly for the encoding graph for B of  $G_1$ , then a fraction  $\frac{1}{b^2}$  of the subcomputations  $G_k^i$  are mutually input-disjoint.

PROOF. Consider the recursion tree of subcomputations computed by  $G_r$ . Let  $P_1$  be the "grandparent" subcomputation of  $G_k^i$  – the subcomputation in the recursion tree two levels above  $G_k^i$  – and suppose  $P_1$  multiplies matrices  $A_1$ by  $B_1$ . Then at least one child subcomputation  $P_2$  of  $P_1$ multiplies matrices  $A_2$  by  $B_2$  such that  $A_2$  shares no metavertices with  $A_1$ . Similarly, at least one child subcomputation of  $P_2$  multiplies matrices  $A_3$  by  $B_3$  such that  $B_3$  shares no meta-vertices with  $B_2$ , and hence with  $B_1$ . Thus at least one subsubcomputation of  $P_1$  is input-disjoint from it.  $P_1$ has  $b^2$  subcomputations two levels down from it, so at least a fraction  $\frac{1}{b^2}$  of all the subcomputations  $G_k^i$  are mutually input-disjoint.  $\Box$ 

Fix a collection C of  $b^{r-k-2}$  mutually input-disjoint subcomputations  $G_k^i$ . Let  $\bar{S}$  be the set of vertices of S on the aforementioned ranks in these subcomputations. Formally, for  $v \in S$  we let  $v \in \bar{S}$  if both conditions below are met:

- 1. v lies on one of the following ranks: rank k of the decoding graph of  $G_r$ , rank r-k of the encoding graph of  $G_r$  that encodes A, or rank r-k of the encoding graph of  $G_r$  that encodes B.
- 2. The subcomputation  $G_k^i$  that v lies in (necessarily as an input or output of) is in C.

Divide the sequence of vertex computations into the smallest segments such that for each segment S we have  $|\bar{S}| \ge 36M$ . Let  $S_i$  be the subset of S in  $G_k^i$  and  $\bar{S}_i$  be the subset of  $\bar{S}$  in  $G_k^i$ . Note that if  $G_k^i$  is not one of the chosen input-disjoint subcomputations then  $\bar{S}_i = \emptyset$ . Intuitively, only the vertices in  $\bar{S}$  "count" towards our I/O lower bound, regardless of how many other vertices lie in S, and we choose our segment divisions such that each segment has enough counted vertices. See Figure 5.

Note that if the condition of Lemma 1 is not met, then the algorithm never computes linear combinations of one of the input matrices. It is well known that any matrix Figure 5: The overall idea of the main proof. For simplicity only one encoding graph is explicitly drawn. The set S is shown in blue. Note that only the elements on rank k of the decoding graph and rank r - k of the encoding graphs in input-disjoint  $G_k^i$ s lie in  $\overline{S}$ . A typical boundary-crossing path in  $G_k^3$ is shown. (Not shown) The two vertices of the path on the bottom rank of  $G_k^3$  lie in different encoding graphs.



multiplication algorithm that computes linear combinations of only one of the input matrices performs no better than naive matrix multiplication and so does not have  $o(n^3)$  arithmetic complexity (i.e., is not a fast matrix multiplication algorithm). Thus from now on we assume the condition of Lemma 1 is met.

Second, we show that our choice of partitioning the sequence of vertex computations into segments S exists. If meta-vertices contained multiple input and/or output vertices counted in  $\bar{S}$ , then including into S the next vertex v in the sequence of vertex computations – which by definition also includes into S every vertex in the same meta-vertex as v – could increase this count by more than one.

LEMMA 2. If  $G_k^i$  and  $G_k^j$  are input-disjoint, then the metavertices corresponding to the inputs and outputs of  $G_k^i$  and  $G_k^j$  are all distinct.

PROOF. Note that the decoding graph of  $G_1$  cannot contain copying. If it did, then in the base case of  $n_0 \times n_0$ matrix multiplication  $C_1 = A_1 B_1$  some outputs would be identically equal, which is not the case. Hence the decoding graph of  $G_r$  contains no copying, and so every output vertex of  $G_k^i$  and  $G_k^j$  is non-duplicated. By definition, the input vertices of  $G_k^i$  and  $G_k^j$  are in distinct meta-vertices, proving the lemma.  $\Box$ 

For the remainder of this proof we will consider, for each i, the entire subcomputation graph  $G_k^i$  (as opposed to just the decoding portion  $D_k^i$ ). We must consider the decoding graph and both encoding graphs of  $G_k^i$  together because the decoding graph by itself, or even the decoding graph plus one encoding graph, may be disconnected. We now state the main theorem used in our proof, whose proof we defer until Section 7. Compare to the routing found in Section 5 between the input and output vertices of each  $D_k^i$ .

THEOREM 2 (ROUTING THEOREM). Let  $G_k$  be the CDAG for  $n_0^k \times n_0^k$  matrix multiplication,  $a = n_0^2$ , and let the encoding graph of the base graph  $G_1$  have 2a inputs and b outputs. Then there exists a  $6a^k$ -routing between the set of inputs of  $G_k$  and the set of outputs of  $G_k$ . Furthermore, every meta-vertex in  $G_k$  is also hit by the routing at most  $6a^k$ times.

For each of the mutually input-disjoint  $G_k^i$  in C, fix a  $6a^k$ -routing guaranteed by the Routing Theorem between the inputs and outputs of  $G_k^i$ . Because the size of the top rank of  $G_k^i$  is  $a^k$  and the size of the bottom rank is  $2a^k$  and  $|\bar{S}_i| \leq |\bar{S}| \leq \frac{1}{2}a^k$ , for every vertex v in  $\bar{S}_i$  there exist at least  $\frac{1}{2}a^k$  paths in the routing that go either:

- 1. between a vertex in S on the bottom rank of  $G_k^i$  and a vertex not in S on the top rank of  $G_k^i$  (if v is on the bottom rank)
- 2. between a vertex not in S on the bottom rank of  $G_k^i$  and a vertex in S on the top rank of  $G_k^i$  (if v is on the top rank).

Thus the routing in  $G_k^i$  contains at least  $\frac{1}{2}a^k|\bar{S}_i|$  boundarycrossing paths; call the set of such paths  $P_i$  and let  $P = \bigcup P_i$ 

be all these boundary-crossing paths in the above routings for all input-disjoint  $G_k^i$ . Then  $|P| \ge \sum \frac{1}{2}a^k |\bar{S}_i| = \frac{1}{2}a^k |\bar{S}|$ .

By the Routing Theorem every meta-vertex contained entirely within  $G_k^i$  is hit by the routing at most  $6a^k$  times. No meta-vertex in  $G_k^i$  extends beneath the bottom rank of  $G_k^i$ , and so every meta-vertex in  $G_r$  intersects at most one of the mutually input-disjoint  $G_k^i$ . Therefore every meta-vertex in  $G_r$  is hit at most  $6a^k$  times by the paths in P.

Let S' be the set of meta-vertices represented by S, and recall that  $\delta'(S')$  denotes all meta-vertices adjacent to S'that are not in S' itself. Then

$$|\delta'(S')| \ge \frac{\frac{1}{2}a^k|\bar{S}|}{6a^k} = \frac{1}{12}|\bar{S}|$$
(2)

This is a more general analogue of Equation 1.

Every meta-vertex adjacent to S necessarily contributes one to the I/Os due to computing S, except possibly for those meta-vertices already in memory (at most M) and those that need not be written to cache (at most M). Because  $|\bar{S}| = 36M$ , we have  $|\delta'(S')| \ge 3M$ , and so computing S requires at least M I/Os.

As indicated above, because  $G_r$  has  $o(n^3)$  multiplications we may apply Lemma 1. Because rank k of the decoding graph of  $G_r$  and rank r - k of the encoding graphs of  $G_r$ together have size  $3a^kb^{r-k}$  and  $\frac{1}{b^2}$  of these vertices are in mutually input-disjoint subcomputations  $G_k^i$ , the total I/O from computing  $G_r$  is at least

$$\left\lfloor \frac{\frac{1}{b^2} 3a^k b^{r-k}}{36M} \right\rfloor \cdot M = \Omega\left(b^r \left(\frac{a}{b}\right)^k\right) = \Omega\left(|V(G_r)| \frac{M}{M^{\log_a b}}\right)$$
$$= \Omega\left(\left(\frac{n}{\sqrt{M}}\right)^{2\log_a b} \cdot M\right)$$

as long as  $M \leq o(n^2)$  (which guarantees that  $36M \leq \frac{1}{h^2} 3a^k b^{r-k}$  and  $k \leq r-2$ ).

In the parallel case, we apply the above argument to a processor that computes an above-average number of vertices of  $\overline{S}$ , yielding a factor of  $\frac{1}{P}$  as in [2]. The cache-independent result comes from instead picking  $k = \Theta\left(\log_b \frac{n^{\omega_0}}{P}\right)$  and letting S represent the computations performed by just one processor. This proves Theorem 1.  $\Box$ 

## 7. PROOF OF THE ROUTING THEOREM

In this section we prove Theorem 2. Let  $G_k$  be the CDAG for a square Strassen-like matrix multiplication algorithm for C = AB, let *Out* be the set of outputs of  $G_k$  (corresponding to entries of C), In be the set of inputs,  $In_A$  be the set of inputs to the encoding graph for A within  $G_k$ , and  $In_B$ be the inputs to the encoding graph for B. Then |Out| = $|In_A| = |In_B| = a^k = n_0^{2k}$ . For  $v \in In$  and  $w \in Out$ , we say that the input-output pair (v, w) is a *quaranteed dependence* if in any correct matrix multiplication algorithm there exists a chain from v to w, or equivalently if the output element corresponding to w explicitly depends on the input element corresponding to v. It is clear that if  $v \in In_A$  represents the input  $a_{ij}$  and w represents the output  $c_{i'j'}$  then there is a guaranteed dependence between v and w if and only if i = i', and similarly if  $v \in In_B$  represents the input  $b_{ij}$ , then there is a guaranteed dependence between v and w if and only if j = j'.

To prove the Routing Theorem we will combine the following two lemmas, whose proofs follow in the succeeding sections:

LEMMA 3. Let  $F \subseteq V(G_k) \times V(G_k)$  be the set of all guaranteed dependencies (v, w) of  $G_k$  with  $v \in In$  and  $w \in Out$ . Then there exists a  $2n_0^k$ -routing for F in  $G_k$  consisting only of chains.

Intuitively, we can route chains between all pairs of input and output vertices where a chain is guaranteed to exist while using no vertex more than  $2\sqrt{a^k}$  times. That every path of the routing is a chain is not necessary to complete the proof of the Routing Theorem.

LEMMA 4. Fix a routing for F, where F is as defined in Lemma 3. Then there exists a routing between In and Out such that every path in the routing consists of the concatenation of chains in F – some reversed in direction – such that each chain in F is used  $3n_0^k$  times.

In other words, given any way of routing chains between all guaranteed dependencies, we can combine those chains, backwards and forwards, to give a path between every input and every output vertex while not using any such chain more than  $3\sqrt{a^k}$  times.

Given these lemmas, the proof is simple:

PROOF OF THE ROUTING THEOREM. By Lemma 3, fix a  $2n_0^k$ -routing  $R_0$  for the set of guaranteed dependencies F. By Lemma 4, there exists a routing R between the inputs and outputs of  $G_r$  composed of concatenations of chains (some reversed) in  $R_0$  such that every chain in  $R_0$  is used at most  $3n_0^k$  times. Thus in the routing R every vertex of G is used at most  $2n_0^k \cdot 3n_0^k = 6a^k$  times, and so R is a  $6a^k$ -routing, as desired.

Because every meta-vertex is an upward-facing subtree (see Figure 2), any path hitting a meta-vertex also hits the root vertex of the meta-vertex. Hence every meta-vertex is also hit at most  $6a^k$  times.  $\Box$ 

### 7.1 Proof of Lemma 4

In this section we prove the second, significantly easier, lemma. The proof of this lemma is constructive, yielding an explicit scheme for routing chains between all inputs and outputs given a routing for all guaranteed dependencies. This lemma holds for any correct matrix multiplication algorithm based only on the definition of matrix multiplication.

PROOF OF LEMMA 4. For an input vertex v of  $G_k$  and output vertex w corresponding to element  $c_{i'j'}$  of C, suppose first that  $v \in In_A$ . Let v then represent element  $a_{ij}$  of A. We form the following sequence of guaranteed dependencies:

$$a_{ij} \rightarrow c_{ij'} \rightarrow b_{jj'} \rightarrow c_{i'j'}$$

That is,  $(a_{ij}, c_{ij'})$  is a guaranteed dependence,  $(b_{jj'}, c_{ij'})$  is a guaranteed dependence, and  $(b_{jj'}, c_{i'j'})$  is a guaranteed dependence. Note that every guaranteed dependence in this chain involves 3 out of the 4 variables i, i', j, and j'. Hence as i, j, i', and j' vary between 1 and  $n_0^b$ , each guaranteed dependence above is used  $n_0^b$  times, once for each value of the missing variable (for each time it appears in the above sequence). For example, for any i, j, and j', the guaranteed dependence between  $a_{ij}$  and  $c_{ij'}$  is used exactly once for every  $1 \leq i' \leq n_0^b$ . See Figure 6 for another interpretation of this pattern.

Similarly, if  $v \in In_B$  let v correspond to element  $b_{ij}$  of B. The following sequence of guaranteed dependencies has the same properties:

$$b_{ij} \to c_{i'j} \to a_{i'i} \to c_{i'j'}$$

Amongst both these sequences, each guaranteed dependence between an element of A and one of C is used exactly  $3 \cdot n_0^6$  times and similarly for every guaranteed dependence between B and C. This proves Lemma 4.  $\Box$ 

Note that these sequences are not unique. When routing  $a_{ij}$  to  $c_{i'j'}$ , any sequence of the form

$$a_{ij} \to c_{ij'} \to b_{j'} \to c_{i'j'}$$

where the blank is any value forms a set of sequences of guaranteed dependencies. However, unless the values that the blank takes are well-distributed over j for all choices of i, i', and j', this sequence will not have the desired property. This explains the odd use of j as a row index, and similarly the use of i as a column index when routing  $b_{ij}$  to  $c_{i'j'}$ .

Figure 6: The sequence of guaranteed dependencies between  $a_{ij}$  and  $c_{i'j'}$  shown as elements in the matrices A, B, and C. Note the use of j as a row index.



## 7.2 Proof of Lemma 3

This lemma is significantly harder to prove. We use the following overall strategy: In order to prove there exists a  $2n_0^k$ -routing between all guaranteed dependencies, we show there exists a  $n_0$ -routing of guaranteed dependencies in the subgraph of  $G_1$  formed by the decoding graph together with the encoding graph for A; by the recursive structure of  $G_k$ , this is sufficient to prove it in general. Define a *middle-rank* vertex of  $G_1$  to be a vertex on the top rank of the encoding graph of A. To show the lemma for this  $\frac{2}{3}$  of  $G_1$ , we show a (several-to-one) matching between guaranteed dependencies and middle-rank vertices on some chain satisfying the dependence. By assumption, every vertex representing a linear combination of elements of A is adjacent to exactly one multiplication vertex; thus a routing of guaranteed dependencies that uses each middle-rank vertex at most  $n_0$  times also uses each multiplication vertex at most  $n_0$  times.

We will prove the existence of this matching via a version of Hall's Matching Theorem. In order to apply this theorem, we will need to show that for every set of d guaranteed dependencies, there exist chains between those dependencies collectively hitting at least  $\frac{d}{n_0}$  middle-rank vertices. We demonstrate that if this is not the case, then setting some entries of the  $n_0 \times n_0$  input matrix A to be identically 0 results in an algorithm that correctly computes many of the guaranteed dependencies between C and A using relatively few multiplications. Finally, we show that this implies the existence of an algorithm for multiplying a  $n_0 \times n_0$  matrix by a length  $n_0$  vector in fewer than  $n_0^2$  operations, which is known to be impossible [15]. This will conclude the proof.

Let  $G'_k$  be the induced subgraph of  $G_k$  containing the vertices from the decoding graph of  $G_k$  and the encoding graph of  $G_k$  for A (excluding only the encoding graph for B). Let F' be the subset of F with both vertices lying in  $G'_k$ , that is the set of guaranteed dependencies (v, w) between inputs v of A and outputs w of C. For simplicity, we simply call F' the guaranteed dependencies of  $G'_k$ . We now consider m-routings for the set of guaranteed dependencies (that is, F') of  $G'_k$ . It then suffices to find an  $a^k$ -routing of guaranteed dependencies in  $G'_k$ .

CLAIM 2. If there exists an m-routing for the guaranteed dependencies of  $G'_1$ , then there exists an  $m^k$ -routing for the guaranteed dependencies of  $G'_k$ .

PROOF. This lemma follows from the recursive structure of  $G'_k$ . Intuitively, the graph  $G'_k$  is formed by placing bcopies of  $G'_{k-1}$  in parallel, connecting up their inputs with  $a^{k-1}$  copies of the encoding graph for A, and connecting up their outputs with  $a^{k-1}$  copies of the decoding graph for C. See Figure 7. In other words, take  $a^{k-1}$  copies of  $G'_1$  and replace their middle two ranks with copies of  $G'_{k-1}$ . Any number of copies of  $G'_1$  in parallel still have an m-routing for guaranteed dependencies, and replacing their middle ranks effectively replaces a pair of adjacent vertices on the middle ranks with a guaranteed dependence in  $G'_{k-1}$ . Thus if there exists an  $m^{k-1}$ -routing for  $G_{k-1}$  then there exists an  $m^k$ routing for  $G_k$ . The claim then follows by induction.  $\Box$ 

Therefore it will suffice to prove the existence of an  $n_0$ routing for the guaranteed dependencies of  $G'_1$ . We now apply a version of Hall's Matching Theorem: Figure 7: The construction of  $G'_k$  from *b* copies of  $G'_{k-1}$ . A pair of adjacent vertices on the middle two ranks is replaced with a guaranteed dependence in one of the  $G'_{k-1}$ .



THEOREM 3 (HALL'S MATCHING THEOREM). (Many-toone version) Let G = (X, Y) be a bipartite graph and for  $D \subseteq V(G)$  let N(D) denote the set of neighbors of D in G. If for every  $D \subseteq X$  we have  $|N(D)| \ge \frac{|D|}{p}$ , then there exists a many-to-one matching between X and Y such that every vertex in X is used exactly once and every vertex in Y is used at most p times.

This theorem follows from the standard form of Hall's Matching Theorem by simply duplicating all vertices in Y p times.

We now construct a graph H = (X, Y) to which to apply Theorem 3. For every guaranteed dependence (v, w) in  $G'_1$ (with v an input representing an element of A and w an output representing an element of C), define a corresponding vertex in X. Let Y be the set of middle-rank vertices of  $G_1$ : all vertices on the top rank of the encoding graph for A. It suffices to assign to each guaranteed dependence in Xa middle-rank vertex from Y through which its chain may pass. To this end, if  $x \in X$  corresponds to the guaranteed dependence (v, w) and  $y \in Y$  corresponds to the middlerank vertex t, let there be an edge between x and y if there exists some chain between v and w passing through t. See Figure 8.

Figure 8: The vertices shown in red are those adjacent to the vertex in H corresponding to the guaranteed dependence (v, w), where v corresponds to the input  $a_{12}$  of A and w corresponds to the output  $c_{11}$ of C. The graph shown is the  $G'_1$  for Strassen's algorithm.



LEMMA 5. For any set  $D \subseteq X$ , we have  $|N(D)| \ge \frac{|D|}{n_0}$ .

From Lemma 5, the proof of Lemma 3 follows, and thus our main result:

PROOF OF LEMMA 3. By Hall's Matching Theorem (Theorem 3), there exists a many-to-one matching from X to Yusing every vertex in Y at most  $n_0$  times. Fix such a matching. For every guaranteed dependence (v, w) of  $G'_1$ , simply route a chain through the vertex of Y that (v, w) is matched with. Every vertex on the middle two ranks of  $G'_1$  is thus hit at most  $n_0$  times. Every vertex on the top and bottom ranks of  $G'_1$  is hit exactly  $n_0$  times by any routing for guaranteed dependencies that uses only chains, because in  $n_0 \times n_0$  matrix multiplication every element of A influences  $n_0$  elements of C, and every element of C depends on  $n_0$  elements of A. Thus there exists a  $n_0$ -routing for the guaranteed dependencies in  $G'_1$ , and so by Claim 2 there exists a  $n_0^k$ -routing for the guaranteed dependencies of  $G'_k$ . The same holds for the induced subgraph of  $G_1$  consisting of the decoding graph together with the encoding graph for B, yielding a  $2n_0^k$ -routing for the guaranteed dependencies of  $G_k$ .  $\Box$ 

#### 7.3 Proof of Lemma 5

Finally, we prove Lemma 5 to complete the proof of the Routing Theorem and thus our main result, Theorem 1:

PROOF OF LEMMA 5. Suppose by way of contradiction that for some subset  $D \subseteq X$  of guaranteed dependencies in  $G'_1$  we have  $|N(D)| < \frac{|D|}{n_0}$ . Recall that a guaranteed dependence occurs between the vertex representing  $a_{ij}$  and the vertex representing  $c_{i'j'}$  exactly when i = i'. We may thus partition D by the choice of i: let  $D_i$  be the subset of D consisting of guaranteed dependencies between  $a_{ij}$  and  $c_{ij'}$  for some j and j'. Because  $1 \leq i \leq n_0$ , for some i we have  $|D_i| \geq \frac{|D|}{n_0}$ . Since  $N(D_i) \subseteq N(D)$ , we have  $|N(D_i)| < \frac{|D|}{n_0} \leq |D_i|$ . In other words, the set of guaranteed dependencies  $D_i$  is computed using fewer than  $|D_i|$ multiplication vertices.

We now demonstrate that this is impossible by using this structure to create a matrix-vector multiplication algorithm that requires fewer than  $n_0^2$  multiplications. For fixed  $D_i$ , define the computation graph  $G_1^{\circ}$  as follows:  $G_1^{\circ}$  is the induced subgraph of  $G_1$  containing as inputs vertices corresponding to all the elements of B and their linear combinations, the elements  $a_{ij}$  of A for all j, and the elements  $c_{ij'}$  of C for all j'.  $G_i^{\circ}$  additionally contains all the middle-rank vertices in  $N(D_i)$  and all vertices on the bottom rank of the decoding graph.  $G_1^{\circ}$  may now contain "useless" vertices – we draw  $G_1^{\circ}$  with these vertices additionally removed, but it does not matter for the bounds in this proof.

By the structure of  $G_1$ , every multiplication vertex multiplies a linear combination  $\sum_{i,j} \lambda_{ij}^A a_{ij}$  by a linear combination  $\sum_{i,j} \lambda_{ij}^B b_{ij}$  for some coefficients  $\lambda_{ij}^A$  and  $\lambda_{ij}^B$  in the ground field F ( $\mathbb{R}$  or  $\mathbb{C}$ ). We consider linear combinations of the  $a_{ij}$ s

F (K of C). We consider linear combinations of the  $a_{ij}$ s with coefficients in  $F[b_{11}, b_{12}, \ldots, b_{n_0n_0}]$ . In other words, consider  $b_{ij}$ s to be coefficients and  $a_{ij}$ s to be variables. For  $1 \leq j \leq n_0$ , let  $a_{ij}$  and  $c_{ij}$  be the inputs and outputs of  $G_1^{\circ}$  respectively. Note that for all  $1 \leq j, j' \leq n_0, c_{ij}$  depends on  $a_{ij'}$ . We now define a boolean-valued function f that represents whether the coefficient of each input is correct in each output: For  $1 \leq j, j' \leq n_0$ , define f(j, j') to be 1

Figure 9:  $G_1^{\circ}$  for Strassen's algorithm when i = 2and  $D_2 = \{(a_{21}, c_{21}), (a_{21}, c_{22}), (a_{22}, c_{22})\}$ . The crossedout vertices are those removed from  $G_1$  to construct this reduced computation graph  $G_1^{\circ}$ . Because the guaranteed dependence  $(a_{22}, c_{21})$  is not included in  $D_2$ , the vertex crossed out in blue is removed, and so  $G_1^{\circ}$  does not quite compute vector-matrix multiplication; the coefficient of  $a_{22}$  in the computation of  $c_{21}$  may not be correct.



exactly when the coefficient of  $a_{ij'}$  in  $c_{ij}$  is its correct value for matrix multiplication, namely  $b_{j'j}$ , and otherwise 0.

Let  $n_f$  denote the number of pairs (j, j') with  $1 \leq j, j' \leq n_0$  at which f takes the value 1 – that is, the number of coefficients correctly set by  $G_1^{\circ}$ . By the definition of  $G_1^{\circ}$  relative to the matching graph H, we have  $n_f \geq |D_i|$ : If the guaranteed dependence of  $c_{ij}$  on  $a_{ij'}$  is represented in  $D_i$ , then the coefficient of  $a_{ij'}$  in  $c_{ij}$  must be "correct" for matrix multiplication, since, by definition of  $G_1^{\circ}$ , there exists no chain between the vertices corresponding to  $c_{ij}$  and  $a_{ij'}$  contained in  $G_1$  (which correctly computes matrix multiplication) but not in  $G_1^{\circ}$ .

Finally, we use  $G_1^{\circ}$  to construct a new, correct, vectormatrix multiplication algorithm. Define  $\bar{G}_1^{\circ}$  to be the CDAG formed as follows: to the CDAG  $G_1^{\circ}$  add  $n_0^2 - n_f$  multiplication vertices, one for each pair (j, j') for which f(j, j') = 0. For  $1 \leq j, j' \leq n_0$  let the coefficient of  $a_{ij'}$  in  $c_{ij}$  computed by  $G_1^{\circ}$  be  $x_{j'j} \in F[b_{11}, b_{12}, \ldots, b_{n_0n_0}]$  – a linear combination of the "coefficients"  $b_{ij}$ . For each such j and j' at which f(j, j') = 0, use a multiplication vertex to compute  $a_{ij'} (b_{j'j} - x_{j'j})$  and add it to the output vertex representing  $c_{ij}$ . In other words, for every incorrect dependence of  $c_{ij}$  on  $a_{ij'}$  we may use a single multiplication vertex to "fix" the dependence. Now  $\bar{G}_1^{\circ}$  correctly computes  $n_0 \times n_0$  vectormatrix multiplication.  $G_1^{\circ}$  contained fewer than  $|D_i|$  multiplication vertices and we added at most  $n_0^2 - n_f$ , so  $\bar{G}_1^{\circ}$  has  $< |D_i| + n_0^2 - n_f \leq |D_i| + n_0^2 - |D_i| = n_0^2$  multiplication vertices. Thus we have constructed a correct algorithm for computing  $n_0 \times n_0$  vector-matrix multiplication using fewer than  $n_0^2$  multiplications, which is known to be impossible [15]. This concludes the proof of Lemma 5 and hence of our main result Theorem 1.  $\Box$ 

We state the result we obtained in the proof of Lemma 5 as its own Lemma:

LEMMA 6. Let  $G_1^{\circ}$  be a CDAG with inputs  $a_{ij}$  and  $b_{ij}$  and outputs  $c_{ij}$  for  $1 \leq i, j \leq n_0$  where each  $c_{ij}$  is computed as a product of linear combinations of the  $a_{ij}$  and  $b_{ij}$ . If for d pairs (j, j'),  $1 \leq j, j' \leq n_0$ , the coefficient of  $a_{ij'}$  in  $c_{ij}$  is  $b_{j'j}$ , then  $G_1^{\circ}$  uses at least d multiplications.

# 8. CONCLUSION

We have proven optimal lower bounds for the I/O-complexity of any Strassen-like square matrix multiplication algorithm in which every linear combination in the base graph is used in only one multiplication by proving the existence of a routing between the inputs and outputs of such an algorithm that uses every intermediate computation vertex relatively few times. The proof generalizes easily to algorithms composed of different base graphs, as long as each base graph performs square matrix multiplication with 2a inputs and b subcomputations and satisfies the conditions of Lemma 1. This bound holds regardless of the form of the base graph(s), including those that have disconnected encoding or decoding pieces and those that perform multiple copying. Our technique provides a novel alternative to the edge expansion argument in [6] that applies to less straightforward recursive computation graphs.

We believe that the assumption that every linear combination is used in only one multiplication can also be lifted. Without this assumption Lemma 5 no longer holds; vertices representing linear combinations used in multiple multiplications may require too many paths routed through them. Thus a more general approach to routing guaranteed dependencies is required. This difficulty can be overcome by routing paths in response to the choice of S, where paths are now allowed to "jump" to other vertices on the same rank of  $G_k$  that have the same membership in S. We believe it can be shown that this optimization does not decrease the number of boundary-crossing edges and still results in every vertex lying on at most  $6a^k$  "generalized" paths, thus extending our result to all fast Strassen-like matrix multiplication algorithms.

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### **10. REFERENCES**

- G. Ballard, E. Carson, J. Demmel, M. Hoemmen, N. Knight, and O. Schwartz. Communication lower bounds and optimal algorithms for numerical linear algebra. Acta Numerica, 23:1–155, 5 2014.
- [2] G. Ballard, J. Demmel, O. Holtz, B. Lipshitz, and O. Schwartz. Brief announcement: strong scaling of matrix multiplication algorithms and memory-independent communication lower bounds. In Proc. 24th ACM Symposium on Parallelism in Algorithms and Architectures (SPAA), SPAA '12, pages 77–79, New York, NY, USA, 2012. ACM.
- [3] G. Ballard, J. Demmel, O. Holtz, B. Lipshitz, and O. Schwartz. Communication-optimal parallel algorithm for Strassen's matrix multiplication. *Proceedings of the 24th ACM Symposium on Parallelism in Algorithms and Architectures, SPAA* 2012, 2012.
- [4] G. Ballard, J. Demmel, O. Holtz, B. Lipshitz, and O. Schwartz. Graph expansion analysis for communication costs of fast rectangular matrix

multiplication. Design and Analysis of Algorithms, 7659:13–36, 2012.

- [5] G. Ballard, J. Demmel, O. Holtz, and O. Schwartz. Minimizing communication in numerical linear algebra. SIAM J. Matrix Anal. & Appl., 32(3):866–901, 2011.
- [6] G. Ballard, J. Demmel, O. Holtz, and O. Schwartz. Graph expansion and communication costs of fast matrix multiplication. *Journal of the ACM*, 59(6), 2012.
- [7] G. Bilardi, A. Pietracaprina, and P. D'Alberto. On the space and access complexity of computation dags. Proceedings of the 26th International Workshop on Graph-Theoretic Concepts in Computer Science, London, UK, pages 47–58, 2000.
- [8] D. Bini, M. Capovani, F. Romani, and G. Lotti.  $o(n^{2.7799})$  complexity for  $n \times n$  approximate matrix multiplication. *Information processing letters*, 8(5):234–235, 1979.
- [9] M. Christ, J. Demmel, N. Knight, T. Scanlon, and K. A. Yelick. Communication lower bounds and optimal algorithms for programs that reference arrays - part 1. Technical Report UCB/EECS-2013-61, EECS Department, University of California, Berkeley, May 2013.

- [10] J. W. Hong and H. T. Kung. The red-blue pebble game. STOC 1981: Proceedings of the thirteenth annual ACM symposium on theory of computing, pages 326–333, 1981.
- [11] J. Hopcroft and L. Kerr. On minimizing the number of multiplications necessary for matrix multiplication. *SIAM Journal on Applied Mathematics*, 20(1):30–36, 1971.
- [12] D. Irony, S. Toledo, and A. Tiskin. Communication lower bounds for distributed-memory matrix multiplication. J. Parallel Distrib. Comput., 64(9):1017–1026, 2004.
- [13] L. H. Loomis and H. Whitney. An inequality related to the isoperimetric inequality. Bulletin of the American Mathematical Society, 55(10), 1949.
- [14] J. Savage. Space-time tradeoffs in memory hierarchies. Technical report, Brown University, Providence, RI, USA, 1994.
- [15] S. Winograd. On the number of multiplications required to compute certain functions. *Proceedings of* the National Academy of Science, 58(5), 1967.
- [16] C.-Q. Yang and B. Miller. Critical path analysis for the execution of parallel and distributed programs. *Proceedings of the 8th International Conference on Distributed Computing Systems*, pages 366–373, 1988.