Optimal Sampling Algorithms for Block Matrix Multiplication*

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Abstract

In this paper, we investigate the randomized algorithms for block matrix multiplication from random sampling perspective. Based on the A-optimal design criterion, the optimal sampling probabilities and sampling block sizes are obtained. To improve the practicability of the block sizes, two modified ones with less computation cost are provided. With respect to the second one, a two step algorithm is also devised. Moreover, the probability error bounds for the proposed algorithms are given. Extensive numerical results show that our methods outperform the existing one in the literature.

Keywords: Optimal sampling, Block matrix multiplication, A-optimal design criterion, Two step algorithm, Probability error bounds

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1. Introduction

As we know, matrix multiplication is a classical problem in numerical linear algebra. The algorithms of this problem are well-known and can be found in any book on matrix computations, see e.g. [1]. However, in the age of big data, these famous algorithms have been encountered enormous challenges because of their computation cost. So, some scholars introduced the randomized ideas to matrix multiplication and proposed some randomized algorithms for this problem.

To the best of our knowledge, Cohen and Lewis [2] first applied the randomized idea to approximate matrix multiplication. In 2006, motivated by a fast sampling algorithm for low-rank approximations given in [3], Drineas et al. [4] proposed the now-famous randomized algorithm for

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matrix multiplication called the BasicMatrixMultiplication algorithm. It picks the outer products using the nonuniform sampling probabilities based on the norms of columns and rows of the involved matrices $M$ and $N$, respectively, that is, the following probabilities

$$p_i = \frac{\|M^{(i)}\|_2 \|N^{(i)}\|_2}{\sum_{i=1}^n \|M^{(i)}\|_2 \|N^{(i)}\|_2}, \quad i = 1, \cdots, n,$$

where $M^{(i)}$ denotes the $i$-th column of $M \in \mathbb{R}^{m \times n}$, $N^{(i)}$ stands for the $i$-th row of $N \in \mathbb{R}^{n \times p}$, and $\| \cdot \|_2$ represents the Euclidean norm of a vector. The specific algorithm is given in Algorithm 1.

Later, the BasicMatrixMultiplication algorithm was extended to the block version by Wu [5]. That is, a set of submatrices were sampled by using the following sampling probabilities

$$p_k = \frac{\|M_k N_k\|_F}{\sum_{k=1}^K \|M_k N_k\|_F}, \quad k = 1, \cdots, K,$$

where $M_k \in \mathbb{R}^{m \times n_k}$ represents the $k$-th block of $M = \begin{bmatrix} M^1 & M^2 & \cdots & M^K \end{bmatrix}$, $N_k \in \mathbb{R}^{n_k \times p}$ symbolizes the $k$-th block of $N^T = \begin{bmatrix} N^T_1 & N^T_2 & \cdots & N^T_K \end{bmatrix}$, and $\| \cdot \|_F$ denotes the Frobenius norm of a matrix. In 2019, Chang et al. [6] proposed another block version of the BasicMatrixMultiplication algorithm with the following sampling probabilities

$$p_k = \frac{\| \sum_{k' \in \mathcal{K}} M_k N_k\|_F}{\sum_{k' \in \mathcal{K}} \| \sum_{k' \in \mathcal{K}} M_k N_k\|_F}, \quad k = 1, \cdots, K,$$

where $\mathcal{K} \subset \{1, 2, 3, \cdots, K\}$ and $\mathcal{K}'$ denote the subsets of $\{1, 2, 3, \cdots, K\}$. Recently, the following sampling probabilities

$$p_k = \frac{\|M_k\|_F \|N_k\|_F}{\sum_{k=1}^K \|M_k\|_F \|N_k\|_F}, \quad k = 1, \cdots, K$$

is, a set of submatrices were sampled by using the following sampling probabilities

\begin{algorithm}[h]
\caption{BasicMatrixMultiplication Algorithm [4]}
\begin{algorithmic}
\State \textbf{Input:} $M \in \mathbb{R}^{m \times n}$, $N \in \mathbb{R}^{n \times p}$, the number of sampling $c \in \mathbb{Z}^+$ such that $1 \leq c \leq n$, and \{\(p_i\)\}_{i=1}^n$ given as (1).
\State \textbf{Output:} $C \in \mathbb{R}^{m \times c}$ and $D \in \mathbb{R}^{c \times p}$.
\State 1. for $t = 1$ to $c$,
\State \hspace{0.5em} (a) sample $i_t \in \{1, \cdots, n\}$ with $\Pr(i_t = s) = p_s$, $s = 1, \cdots, n$, independently and with replacement.
\State \hspace{0.5em} (b) set $C(t) = M(i_t) \sqrt{cp(i_t)}$, and $D(t) = N(i_t) \sqrt{cp(i_t)}$.
\State 2. return $C$ and $D$.
\end{algorithmic}
\end{algorithm}
were devised for the block matrix multiplication by Charalambides et al. They are easier to compute compared with (2) and (3). In addition, there are some other generalizations of the BasicMatrixMultiplication algorithm and some randomized algorithms for matrix multiplication based on random projection. In particular, a block diagonal random projection method with different block sizes was developed in [12].

In this paper, we consider the randomized algorithms for block matrix multiplication based on random sampling further using the technique of optimal subsampling proposed recently in the field of statistics. Specifically, we derive the optimal sampling probabilities and sampling block sizes by the A-optimal design criterion. Moreover, unlike [5–7], we don’t sample the blocks directly but sample the outer products on each block with the optimal sampling probabilities and sampling block sizes.

The remainder of this paper is organized as follows. The randomized algorithm for block matrix multiplication, optimal sampling probabilities and optimal sampling block sizes are presented in Section 2. In Section 3 we modify the block sizes to make them easier to compute and provide a two step algorithm. Furthermore, the probability error bounds of the corresponding algorithms are also given in Sections 2 and 3 respectively. Extensive numerical experiments are shown in Section 4. Finally, we make the concluding remarks of the whole paper.

2. Randomized Algorithm and Optimal Sampling Criterion

We first rewrite the product of the block matrices $M \in \mathbb{R}^{m \times n}$ and $N \in \mathbb{R}^{n \times p}$ appearing in Section 1 as follows

$$MN = K \sum_{k=1}^{K} M^{k} N_{k} = K \sum_{k=1}^{K} \sum_{i=1}^{n} M^{k(i)} N_{k(i)},$$

where $M^{k(i)}$ is viewed as the $i$-th column of the $k$-th block of $M$ and $N_{k(i)}$ is the $i$-th row of the $k$-th block of $N$. Then, Algorithm 1 is applied to each block. Thus, we have $K$ estimates for the $K$ blocks as follows

$$C^{k} D_{k} = \sum_{t=1}^{c_{k}} C^{k(t)} D_{k(t)} = \sum_{t=1}^{c_{k}} \frac{M^{k(i)} N_{k(i)}}{c_{k} p_{k(i)}}, \quad k = 1, \ldots, K,$$

where $c_{k}$ represents the number of extracted outer products from the $k$-th block, $C^{k(t)} = M^{k(i)}/c_{k} p_{k(i)}$, and $D_{k(t)} = N_{k(i)}/c_{k} p_{k(i)}$ with $p_{k(i)}$ be the sampling probability satisfying $\sum_{i=1}^{n} p_{k(i)} = 1$. Note
that these probabilities as well as the sampling block sizes $c_k$ with $k = 1, \ldots, K$ need to be determined later in this section. Hence, they are undetermined at present. Therefore, the final estimate is

$$CD = \sum_{k=1}^{K} C^k D_k = \sum_{k=1}^{K} \sum_{t=1}^{c_k} C^{k(t)} D_{k(t)} = \sum_{k=1}^{K} \sum_{t=1}^{c_k} \frac{M^{k(i)} N^{k(i)}}{c_k p_{k(i)}}.$$

(7)

The specific algorithm is presented in Algorithm 2.

Algorithm 2 Sampling Algorithm for Block Matrix Multiplication

**Input:** $M \in \mathbb{R}^{m \times n}$ and $N \in \mathbb{R}^{n \times p}$ set as in Section 1, \{${n_k}$\}$_{k=1}^{K}$ such that \(\sum_{k=1}^{K} n_k = n\), \{${c_k}$\}$_{k=1}^{K}$ with $c_k \in \mathbb{Z}^+$ and $1 \leq c_k \leq n_k$ such that \(\sum_{k=1}^{K} c_k = c\) for $c \in \mathbb{Z}^+$, and \{${p_k}$\}$_{i=1}^{n_k}$ with $p_{ki} \geq 0$ such that $\sum_{i=1}^{n_k} p_{ki} = 1$ for $k = 1, \ldots, K$.

**Output:** $C \in \mathbb{R}^{m \times c}$, $D \in \mathbb{R}^{c \times p}$, and $CD$.

1. for $k \in 1, \ldots, K$ do
   $[C^k, D_k]$ = BasicMatrixMultiplication($M^k, N_k, c_k, \{p_k\}_{i=1}^{n_k}$)
2. end
3. $C = \begin{bmatrix} C^1 & C^2 & \ldots & C^K \end{bmatrix}$, $D^T = \begin{bmatrix} D_1^T & D_2^T & \ldots & D_K^T \end{bmatrix}$
4. $CD = \sum_{k=1}^{K} C^k D_k$
5. return $C$, $D$, and $CD$

In the following, we discuss the asymptotic properties of the estimation obtained by Algorithm 2. Based on these asymptotic properties and the A-optimal design criterion, we can construct the optimal sampling probabilities and sampling block sizes. Two conditions and a lemma are first listed as follows.

**Condition 1.**

$$\sum_{k=1}^{K} \frac{1}{c_k^2} \cdot \left[ \sum_{i=1}^{n_k} \frac{|M^{k(h,i)}||N^{k(i,f)}|}{p_{ki}} \right]^2 = o_p(1),$$

(8)

where $M^{k(h,i)}$ with $h = 1, \ldots, m$ and $i = 1, \ldots, n_k$ represent the elements at the $(h, i)$-th position of the $k$-th block of $M$, and $N^{k(i,f)}$ with $f = 1, \ldots, p$ and $i = 1, \ldots, n_k$ denote the $(i, f)$-th position of the $k$-th block of $N$.

**Condition 2.**

$$\sum_{k=1}^{K} \sum_{i=1}^{n_k} \frac{(M^{k(h,i)})^2(N^{k(i,f)})^2}{\sqrt{c_k p_{ki}}} = O_p(1).$$

(9)
Lemma 1. The matrices $C$ and $D$ constructed by Algorithm 2 satisfy
\[ E[(CD)_{(h,f)}] = (MN)_{(h,f)} \]  
(10)
and
\[ \text{Var}[(CD)_{(h,f)}] = \sum_{k=1}^{K} \sum_{i=1}^{n_k} \frac{(M_{k(i,i)})^2(N_{k(i,f)})^2}{c{k}p_k} - \sum_{k=1}^{K} \frac{((M_k^kN_k)_{(h,f)})^2}{c_k}. \]  
(11)

Proof. The proof can be completed easily along the line of the proof of [4, Lemma 3].

Now we present the asymptotic distribution of the estimation errors of matrix elements.

Theorem 2. Assume that Conditions 1 and 2 hold and let $c_s = \min_{k=1,\ldots,K} c_k$. Then the matrices $C$ and $D$ constructed by Algorithm 2 satisfy
\[ \frac{(CD)_{(h,f)} - (MN)_{(h,f)}}{\sigma} \xrightarrow{L} N(0, 1), \text{ for } h = 1, \ldots, m \text{ and } f = 1, \ldots, p, \]  
(12)
where $\xrightarrow{L}$ denotes the convergence in distribution, and
\[ \sigma^2 = \sum_{k=1}^{K} \sum_{i=1}^{n_k} \frac{(M_{k(i,i)})^2(N_{k(i,f)})^2}{c_k p_k} - \sum_{k=1}^{K} \frac{((M_k^kN_k)_{(h,f)})^2}{c_k} = O_p((\sqrt{c_s})^{-1}). \]

Proof. Note that
\[
(CD)_{(h,f)} - (MN)_{(h,f)} = \sum_{k=1}^{K} \sum_{i=1}^{c_k} \left( \frac{M_{k(i,i)}N_{k(i,f)}}{c_k p_k} \right)_{(h,f)} - \sum_{k=1}^{K} \sum_{i=1}^{n_k} (M_k^kN_k)_{(h,f)}^{(i,f)} - \sum_{i=1}^{n_k} \frac{(M_k^kN_k)_{(h,f)}^{(i,f)}}{c_k}.
\]

Let $\eta_{k(t)} = \frac{M_{k(i,i)}N_{k(i,f)}}{c_k p_k} - \sum_{i=1}^{n_k} \frac{M_{k(i,i)}N_{k(i,f)}}{c_k} \text{ with } k = 1, \ldots, K \text{ and } t = 1, \ldots, c_k$. Thus, based on Lemma 1, it is easy to deduce that
\[ E[\eta_{k(t)}] = 0 \]  
(13)
and
\[ \text{Var}[\eta_{k(t)}] = \sum_{i=1}^{n_k} \frac{(M_{k(i,i)})^2(N_{k(i,f)})^2}{c_k p_k} - \frac{((M_k^kN_k)_{(h,f)})^2}{c_k^2}. \]  
(14)
Moreover, considering that \( \eta_{k(t)} \) are independent for the given matrices \( M \) and \( N \), by the basic triangle inequality and the Cauchy-Schwarz inequality, for any \( \zeta > 0 \), we have

\[
\sum_{k=1}^{K} \sum_{i=1}^{c_k} E[\eta_{k(t)}^2 I(|\eta_{k(t)}| > \zeta)|M, N] \leq \sum_{k=1}^{K} \sum_{i=1}^{c_k} \frac{1}{\zeta} E[|\eta_{k(t)}|^3|M, N] \\
\leq \sum_{k=1}^{K} \sum_{i=1}^{c_k} \frac{1}{\zeta} E[(\frac{M^k_{(h,i)} N_{k(i,f)}}{c_k p_{k_i}})^3] \\
\leq \sum_{k=1}^{K} \sum_{i=1}^{c_k} \frac{1}{\zeta c_k} \sum_{i=1}^{n_k} |M^k_{(h,i)}|^3 |N_{k(i,f)}|^3 + (n_k \sum_{i=1}^{c_k} |M^k_{(h,i)}||N_{k(i,f)}|)^3 \\
+ 3(n_k \sum_{i=1}^{c_k} |M^k_{(h,i)}||N_{k(i,f)}|) (n_k \sum_{i=1}^{c_k} |M^k_{(h,i)}||N_{k(i,f)}|)^2 + 3 n_k \sum_{i=1}^{c_k} |M^k_{(h,i)}|^2 |N_{k(i,f)}|^2 (n_k \sum_{i=1}^{c_k} |M^k_{(h,i)}||N_{k(i,f)}|) \\
\leq \sum_{k=1}^{K} \sum_{i=1}^{c_k} \frac{8}{\zeta c_k} \left( \sum_{i=1}^{n_k} \frac{|M^k_{(h,i)}||N_{k(i,f)}|}{p_{k_i}} \right)^3 = o_p(1),
\]

where the last equality is from Condition 1. In addition, by (14), we have

\[
\sigma^2 = \sum_{k=1}^{K} \sum_{i=1}^{c_k} \text{Var}[\eta_{k(t)}] \\
= \sum_{k=1}^{K} \sum_{i=1}^{c_k} (\frac{\sum_{i=1}^{n_k} (M^k_{(h,i)})^2 (N_{k(i,f)})^2}{c_k p_{k_i}}) - \sum_{k=1}^{K} (\frac{\sum_{i=1}^{n_k} (M^k_{(h,i)})^2 (N_{k(i,f)})^2}{c_k}) \\
\leq \sum_{k=1}^{K} \sum_{i=1}^{c_k} (\frac{\sum_{i=1}^{n_k} (M^k_{(h,i)})^2 (N_{k(i,f)})^2}{c_k p_{k_i}}) \\
\leq \frac{1}{\sqrt{c_x}} \sum_{k=1}^{K} \sum_{i=1}^{c_k} (\frac{\sum_{i=1}^{n_k} (M^k_{(h,i)})^2 (N_{k(i,f)})^2}{\sqrt{c_k p_{k_i}}}) \\
= O_p((\sqrt{c_x})^{-1}),
\]

where the last inequality is derived by noting \( c_x = \min_{k=1,\cdots,K} c_k \) and the last equality is based on Condition 2. Thus, combining (13), (15) and (16), by the Lindeberg-Feller central limit theorem [17, Proposition 2.27], we get (12).

Remark 1. When \( c_x \to \infty \), the variance \( \sigma^2 \) can be negligible.

Combining the A-optimal design criterion and the sum of asymptotic variances of elements, we can obtain the optimal sampling probabilities \( \{p_{k_i}\}_{i=1}^{n_k} \) with \( k = 1, \cdots, K \) and the optimal sampling block sizes \( \{c_k\}_{k=1}^{K} \) for Algorithm 2.
Theorem 3. For Algorithm 3, the sum of the asymptotic variances,

$$\sum_{h=1}^{m} \sum_{f=1}^{p} \sigma^2$$

attains its minimum when

$$p_{k_i} = \frac{\|M^{k(i)}\|_2 \|N_{k(i)}\|_2}{\sum_{i=1}^{n_k} \|M^{k(i)}\|_2 \|N_{k(i)}\|_2}, \text{ for } k = 1, \cdots, K \text{ and } i = 1, \cdots, n_k,$$

and

$$c_k = c \left( \frac{(\sum_{i=1}^{n_k} \|M^{k(i)}\|_2 \|N_{k(i)}\|_2)^2 - \|M^k N_k\|_F^2}{\sum_{k=1}^{K} ((\sum_{i=1}^{n_k} \|M^{k(i)}\|_2 \|N_{k(i)}\|_2)^2 - \|M^k N_k\|_F^2)} \right)^{\frac{1}{2}}, \text{ for } k = 1, \cdots, K.$$

Proof. Considering

$$\left( \sum_{i=1}^{n_k} \|M^{k(i)}\|_2 \|N_{k(i)}\|_2 \right)^2 - \|M^k N_k\|_F^2 \geq 0$$

and by the Cauchy-Schwarz inequality, it is easy to get

$$\sum_{h=1}^{m} \sum_{f=1}^{p} \sigma^2 = \sum_{k=1}^{K} \sum_{i=1}^{n_k} \frac{\|M^{k(i)}\|_2 \|N_{k(i)}\|_2}{c_k p_{k_i}} - \sum_{k=1}^{K} \frac{\|M^k N_k\|_F^2}{c_k}$$

$$= \sum_{k=1}^{K} \sum_{i=1}^{n_k} p_{k_i} \sum_{i=1}^{n_k} \frac{\|M^{k(i)}\|_2 \|N_{k(i)}\|_2}{c_k p_{k_i}} - \sum_{k=1}^{K} \frac{\|M^k N_k\|_F^2}{c_k}$$

$$\geq \sum_{k=1}^{K} \frac{1}{c_k} \sum_{i=1}^{n_k} \left( \|M^{k(i)}\|_2 \|N_{k(i)}\|_2 \right)^2 - \sum_{k=1}^{K} \frac{\|M^k N_k\|_F^2}{c_k}$$

$$= \sum_{k=1}^{K} \frac{c_k}{c} \sum_{k=1}^{K} \frac{1}{c_k} \left( \sum_{i=1}^{n_k} \left( \|M^{k(i)}\|_2 \|N_{k(i)}\|_2 \right)^2 - \|M^k N_k\|_F^2 \right)$$

$$\geq \sum_{k=1}^{K} \frac{1}{\sqrt{c}} \left( \sum_{i=1}^{n_k} \left( \|M^{k(i)}\|_2 \|N_{k(i)}\|_2 \right)^2 - \|M^k N_k\|_F^2 \right)^{\frac{1}{2}},$$

where the equality in (19) holds if and only if $p_{k_i}$ are proportional to $\|M^{k(i)}\|_2 \|N_{k(i)}\|_2$, i.e., $p_{k_i} = W_1 \|M^{k(i)}\|_2 \|N_{k(i)}\|_2$ for some constant $W_1 \geq 0$, and the equality in the last inequality holds if and only if $c_k = W_2 \left( \sum_{i=1}^{n_k} \|M^{k(i)}\|_2 \|N_{k(i)}\|_2 \right)^2 - \|M^k N_k\|_F^2 \|^\frac{1}{2}$ for some $W_2 \geq 0$. Thus, considering $\sum_{k=1}^{K} c_k = c$ and $\sum_{i=1}^{n_k} p_{k_i} = 1$, the desired results are derived.

Remark 2. It is not a complicated matter to find that

$$\sum_{h=1}^{m} \sum_{f=1}^{p} \sigma^2 = \sum_{h=1}^{m} \sum_{f=1}^{p} \text{Var}[(CD)_{(h,f)}] = \text{E}[(\|MN - CD\|_F^2)],$$
hence, the statistical criterion in Theorem 3 for getting the optimal sampling probabilities and sampling block sizes is equivalent to the optimization criterion used in [4].

Remark 3. Supposing \( v_k \sum_{i=1}^{n_k} \| M_k^{(i)} \|_2 \| N_k^{(i)} \|_2 = \| M_k N_k \|_F \) for \( 0 \leq v_k \leq 1 \), and combining (17) and (18), the sum of asymptotic variances of elements can be rewritten as

\[
\sum_{h=1}^{m} \sum_{f=1}^{p} \sigma^2 = \frac{1}{c} \sum_{k=1}^{K} (1 - v_k^2)^{-\frac{3}{2}} \sum_{i=1}^{n_k} \| M_k^{(i)} \|_2 \| N_k^{(i)} \|_2^2.
\] (20)

Next, we present the error bounds of the estimation obtained by Algorithm 2. To make the analysis more general, we consider a set of sampling probabilities \( \{ p_k \}_{i=1}^{n_k} \) such that

\[
p_k \geq \beta \frac{\| M_k^{(i)} \|_2 \| N_k^{(i)} \|_2}{\sum_{i=1}^{n_k} \| M_k^{(i)} \|_2 \| N_k^{(i)} \|_2}
\]

with a positive constant \( \beta \leq 1 \), which are named as the nearly optimal probabilities.

Theorem 4. Assume \( v_k \sum_{i=1}^{n_k} \| M_k^{(i)} \|_2 \| N_k^{(i)} \|_2 = \| M_k N_k \|_F \) for \( 0 \leq v_k \leq 1 \) and \( \theta_1 \leq 1 - v_k^2 \leq \theta_2 \) with \( 0 \leq \theta_1 \leq \theta_2 \leq 1 \) and \( k = 1, \ldots, K \), and let \( \varphi = \frac{\theta_2 - \theta_1 \beta + \theta_2 \beta_1}{(\theta_2 \theta_1)^{1/4}} \). Then, for Algorithm 2 applied with \( p_k \geq \frac{\beta \| M_k^{(i)} \|_2 \| N_k^{(i)} \|_2}{\sum_{i=1}^{n_k} \| M_k^{(i)} \|_2 \| N_k^{(i)} \|_2} \) for \( \beta \leq 1 \) and \( c_k \) in (18), the sum of the asymptotic variances satisfies

\[
\sum_{h=1}^{m} \sum_{f=1}^{p} \sigma^2 \leq \frac{\varphi^2}{\beta c} \| M \|_F^2 \| N \|_F^2,
\] (21)

and by setting \( \delta \in (0, 1) \) and \( \eta = \varphi + (\frac{\varphi}{\beta_1})^{1/2} \sqrt{(8/\beta) \log(1/\delta)} \),

\[
\| M N - C D \|_F^2 \leq \frac{\eta^2}{\beta c} \| M \|_F^2 \| N \|_F^2
\] (22)
holds with the probability at least \( 1 - \delta \).

Proof. Similar to the proof of [4, Theorem 1], we can derive the desired results. The specific proof is presented in Appendix A.

3. Modification of the Optimal Criterion

Note that calculating (18) requires to figure out the matrix multiplication \( M_k N_k \). This cost may be prohibitive for massive data. In this section, we develop two low-cost alternatives, \( \hat{c}_k \) and \( \tilde{c}_k \), to replace the optimal sampling block size \( c_k \) in (18). Besides, a two step algorithm is also provided with respect to \( \tilde{c}_k \).
3.1. Modification with Adjusting Variance

The size $c_k$ is derived from a small modification in the proof of Theorem 3. That is, we first let

$$\sum_{h=1}^{m} \sum_{f=1}^{p} \sigma^2 = \sum_{k=1}^{K} \sum_{i=1}^{n_k} \frac{\|M^{k(i)}\|_2^2 \|N^{k(i)}\|_2^2}{\hat{c}_k p_k} - \sum_{k=1}^{K} \frac{\|M^{k} N^{k}\|_F^2}{\hat{c}_k} \leq \sum_{k=1}^{K} \sum_{i=1}^{n_k} \frac{\|M^{k(i)}\|_2^2 \|N^{k(i)}\|_2^2}{\hat{c}_k p_k},$$

(23)

and then find two sets $\{\hat{c}_k\}_{k=1}^{K}$ and $\{p_k\}_{i=1}^{n_k}$ to make the above upper bound achieve minimum. Similar to the proof of Theorem 3, we have

$$\hat{c}_k = \frac{1}{\hat{c}^2} \sum_{k=1}^{K} \sum_{i=1}^{n_k} \frac{\|M^{k(i)}\|_2 \|N^{k(i)}\|_2}{\sum_{k=1}^{K} \sum_{i=1}^{n_k} \|M^{k(i)}\|_2 \|N^{k(i)}\|_2}$$

(24)

and $p_k$, as in (17). Obviously, $\hat{c}_k$ is much easier to compute compared with (18).

Below we provide the asymptotic distribution of the estimation errors of matrix elements and probability error bound of $\hat{C} \hat{D}$ constructed by putting (17) and (24) into Algorithm 2. The following conditions are first listed.

**Condition 3.**

$$\frac{1}{\hat{c}^2} \sum_{k=1}^{K} \sum_{i=1}^{n_k} \|M^{k(i)}\|_2 \|N^{k(i)}\|_2^2 = o_p(1).$$

**Condition 4.**

$$\frac{1}{\hat{c}^2} \sum_{k=1}^{K} \sum_{i=1}^{n_k} \|M^{k(i)}\|_2^2 \|N^{k(i)}\|_2 = O_p(1).$$

**Theorem 5.** Assume $\mu_1 L \leq |M_{(h,f)}| \leq \mu_2 L$ and $\mu_1 L \leq |N_{(h,f)}| \leq \mu_2 L$ for $\mu_1 \geq 0$, $\mu_2 \geq 0$ and $L \geq 0$, and set $c_k = \min_{k=1,\ldots,K} \hat{c}_k$. If Conditions 3 and 4 hold, then the matrices $\hat{C}$ and $\hat{D}$ constructed by Algorithm 2 with $p_k$, being as in (17) and $c_k = \hat{c}_k$, satisfy

$$\frac{(\hat{C} \hat{D})_{(h,f)} - (MN)_{(h,f)}}{\sigma} \xrightarrow{L} N(0,1), \text{ for } h = 1, \ldots, m \text{ and } f = 1, \ldots, p,$$

where $\xrightarrow{L}$ denotes the convergence in distribution, and

$$\sigma^2 = \sum_{k=1}^{K} \sum_{i=1}^{n_k} \|M^{k(i)}\|_2 \|N^{k(i)}\|_2 \sum_{k=1}^{K} \frac{1}{c} \sum_{i=1}^{n_k} \frac{(M^{k(i)})^2 (N^{k(i),f})^2}{\|M^{k(i)}\|_2 \|N^{k(i)}\|_2} - \sum_{i=1}^{n_k} \frac{(M^{k} N^{k})_{(h,f),i}}{\|M^{k} N^{k}\|_2 (N^{k(i)}\|_2).$$

**Proof.** The proof can be completed along the line of the proof of Theorem 2.
Theorem 6. Let $\hat{\theta} = (1 - \beta^2(1 - \theta_2))^{1/2}$ with $\theta_2$ given as in Theorem 4. Then, for Algorithm 3 applied with $p_k \geq \frac{\beta \|M^k(i)\|_2 \|N_{k(i)}\|_2}{\sum_{i=1}^K \|M^k(i)\|_2 \|N_{k(i)}\|_2}$ for $\beta \leq 1$ and $c_k = \hat{c}_k$, the sum of the asymptotic variances satisfies

$$\sum_{h=1}^m \sum_{f=1}^p \sigma^2 \leq \frac{\hat{\theta}^2}{\beta C} \|M\|^2_F \|N\|^2_F,$$

and by setting $\delta \in (0, 1)$ and $\eta = \hat{\theta} + \sqrt{(8/\beta) \log(1/\delta)}$,

$$\|MN - \hat{C}\hat{D}\|^2_F \leq \frac{\eta^2}{\beta C} \|M\|^2_F \|N\|^2_F$$

holds with the probability at least $1 - \delta$.

Proof. The proof can be completed along the line of the proof of Theorem 4.

Remark 4. Let $\theta_2 = \theta_1 < 1$ and $\beta = 1$ in Theorem 6 we have $\eta = (\theta_2)^{1/2} + \sqrt{(8/\beta) \log(1/\delta)}$. In this case, the corresponding probability error bound is the same as the one in Theorem 4.

3.2. Modification with the BasicMatrixMultiplication Algorithm

We can use $C^0D^0$ constructed by Algorithm 1 with the same sampling size $[c0/K]$ and a set of sampling probabilities $\{p_{0k}\}_{i=1}^{n_k}$ to approximate $M^kN_k$, where $c0$ denotes the total sample size, and $p_{0k}$, with $i = 1, \ldots, n_k$ are allowed to be uniform probabilities or nonuniform probabilities. Considering that $(\sum_{i=1}^{n_k} \|M^k(i)\|_2 \|N_{k(i)}\|_2)^2 - \|C^0D^0\|^2_F \geq 0$ may not hold, we propose $\tilde{c}_k$ as follows

$$\tilde{c}_k = c \frac{((\sum_{i=1}^{n_k} \|M^k(i)\|_2 \|N_{k(i)}\|_2)^2 - \|C^0D^0\|^2_F)\hat{\theta}^2}{\sum_{i=1}^{n_k} ((\sum_{i=1}^{n_k} \|M^k(i)\|_2 \|N_{k(i)}\|_2)^2 - \|C^0D^0\|^2_F))\hat{\theta}^2}.$$

Based on the above idea, we devise a two step algorithm summarized in Algorithm 3.

Theorem 7. Suppose $\hat{\nu}_k \sum_{i=1}^{n_k} \|M^k(i)\|_2 \|N_{k(i)}\|_2 = \|C^0D^0\|_F$, for $\hat{\nu}_1 \leq 1 - \hat{\nu}_k^2 \leq \hat{\nu}_2$ with $k = 1, \ldots, K$, set $\mu_1$, $\mu_2$ and $L$ as in Theorem 4 and let $c_s = \min_{k=1, \ldots, K} \tilde{c}_k$. If Conditions 3 and 4 hold, then the matrices $\tilde{C}$ and $\tilde{D}$ constructed by Algorithm 3 satisfy

$$(\tilde{C}\tilde{D})_{(h,f)} - (MN)_{(h,f)} \overset{\sigma}{\to} N(0, 1),$$

for $h = 1, \ldots, m$ and $f = 1, \ldots, p$. 

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Algorithm 3 Two Step Algorithm for Block Matrix Multiplication

**Input:** $M \in \mathbb{R}^{m \times n}$ and $N \in \mathbb{R}^{n \times p}$ set as in Section 1, $\{n_k\}_{k=1}^K$ such that $\sum_{k=1}^K n_k = n$, $c \in \mathbb{Z}^+$, $c_0 \in \mathbb{Z}^+$, and $\{p_{0k_i}\}_{i=1}^{n_k}$ with $p_{0k_i} \geq 0$ such that $\sum_{i=1}^{n_k} p_{0k_i} = 1$, $k = 1, \ldots, K$.

**Output:** $\tilde{C} \in \mathbb{R}^{m \times c}$, $\tilde{D} \in \mathbb{R}^{c \times p}$, and $\tilde{C}\tilde{D}$.

**Step 1:**

1. for $k \in 1, \ldots, K$ do
   1. update $[C^{0k}, D^{0k}] = \text{BasicMatrixMultiplication}(M^k, N_k, [c_0/K], \{p_{0k_i}\}_{i=1}^{n_k})$
   2. update $p_{ki} = \frac{\|M^k(i)\|_2\|N_k(i)\|_2}{\sum_{i=1}^{n_k} \|M^k(i)\|_2\|N_k(i)\|_2}$, $i = 1, \ldots, n_k$
   3. end

2. replace $\|M^k N_k\|_2^2$ in (13) by $C^{0k} D^{0k}$, i.e., $\tilde{c}_k = c \frac{\left(\sum_{i=1}^{n_k} \|M^k(i)\|_2\|N_k(i)\|_2\right)^2 - \|C^{0k} D^{0k}\|_F^2}{\sum_{k=1}^K \left(\sum_{i=1}^{n_k} \|M^k(i)\|_2\|N_k(i)\|_2\right)^2 - \|C^{0k} D^{0k}\|_F^2}$

3. return $\tilde{c}_k$ for $k = 1, \ldots, K$, and $p_{ki}$ for $k = 1, \ldots, K$ and $i = 1, \ldots, n_k$

**Step 2:**

1. for $k \in 1, \ldots, K$ do
   $[\tilde{C}^k, \tilde{D}^k] = \text{BasicMatrixMultiplication}(M^k, N_k, \tilde{c}_k, \{p_{ki}\}_{i=1}^{n_k})$
   2. end

3. $\tilde{C} = \begin{bmatrix} \tilde{C}^1 & \tilde{C}^2 & \cdots & \tilde{C}^K \end{bmatrix}$, $\tilde{D}^T = \begin{bmatrix} \tilde{D}_1^T & \tilde{D}_2^T & \cdots & \tilde{D}_K^T \end{bmatrix}$

4. $\tilde{C}\tilde{D} = \sum_{k=1}^K \tilde{C}^k \tilde{D}^k$

5. return $\tilde{C}$, $\tilde{D}$, and $\tilde{C}\tilde{D}$
where \( \xrightarrow{D} \) denotes the convergence in distribution, and

\[
\sigma^2 = \sum_{k=1}^{K} |1 - \hat{v}_k^2| \sum_{i=1}^{n_k} \|M^{(i)}\|_2 \|N^{(i)}\|_2 \sum_{k=1}^{K} \frac{1}{c(1 - \hat{v}_k^2)} \sum_{i=1}^{n_k} \|M^{(i)}\|_2 \|N^{(i)}\|_2 - \sum_{i=1}^{n_k} \|M^{(i)}\|_2 \|N^{(i)}\|_2)
\]

\( = O_p((\sqrt{c}^{-1})^{-1}). \)

**Proof.** The proof can be completed along the line of the proof of Theorem 2.

**Theorem 8.** Assume the same setting as in Theorem 7 and let \( \tilde{\phi} = \theta_2 - \theta_1 \tilde{\hat{\phi}} + \theta_1 \hat{\phi} \) with \( \theta_2 \) given as in Theorem 4. Then, for Algorithm 3 applied with \( p_k \geq \frac{\beta \|M^{(i)}\|_2 \|N^{(i)}\|_2}{\sum_{i=1}^{m_k} \|M^{(i)}\|_2 \|N^{(i)}\|_2} \) for \( \beta \leq 1 \), the sum of the asymptotic variances satisfies

\[
\sum_{h=1}^{m} \sum_{f=1}^{p} \sigma^2 \leq \frac{\beta^2}{\beta c} \|M\|_F^2 \|N\|_F^2,
\]

(28)

and by setting \( \delta \in (0, 1) \) and \( \eta = \tilde{\phi} + (\tilde{\phi} - \theta_1 \hat{\phi}) \sqrt{8/\beta \log(1/\delta)} \), then

\[
\|MN - \tilde{C}D\|_F^2 \leq \frac{\eta^2}{\beta c} \|M\|_F^2 \|N\|_F^2
\]

(29)

holds with the probability at least \( 1 - \delta \).

**Proof.** The proof can be completed along the line of the proof of the proof of Theorem 4.

**Remark 5.** When \( \theta_2 > 1, \theta_1 \leq 1 \) and \( 1 - \theta_2 = o_p(1) \), the bounds in Theorem 8 is a little weaker than the one in Theorem 7.

4. Numerical Experiments

Without loss of generality, we set the sizes of the blocks of the involved block matrices \( M \) and \( N \) to be the same, namely \( n_k = n/K \) for \( k = 1, \cdots, K \). To construct the following matrices \( M \) and \( N \), we let \( m = 26, p = 28, n = 5 \times 10^5, \Sigma_1 = (1 \times 0.7^{(i-j)}) \) with \( 1 \leq i,j \leq m \) and \( \Sigma_2 = (2 \times 0.7^{(i-j)}) \) with \( 1 \leq i,j \leq p. \)

Case I: The \( i \)-th column of \( M \) with \( 1 \leq i \leq m \), \( M^{(i)} \), is generated from a multivariate normal distribution, that is, \( M^{(i)} \sim N(0, \Sigma_1) \). Similarly, set \( N^{(i)} \sim N(0, \Sigma_2) \).

Case II: The \( i \)-th column of \( M \) with \( 1 \leq i \leq m \), \( M^{(i)} \), is generated from a multivariate \( t \) distribution with 1 degree of freedom, that is, \( M^{(i)} \sim t_1(1, \Sigma_1) \). Similarly, set \( N^{(i)} \sim t_1(1, \Sigma_2) \).
For the above matrices, by setting suitable values of $K$, $c0$ and $c$, we do five specific experiments summarized in Table 1 and report the numerical results on accuracy and CPU time in Figures 1-10. Note that all the numerical results are based on 100 replications, and in these figures, SSM denotes the method from [7], whose sampling probabilities are given in (4), and other notations for the methods are introduced in Table 2.

| Number | Comparison | $c$          | $K$          | $c0$       | Results               |
|--------|------------|--------------|--------------|------------|-----------------------|
| 1      | Algorithm 2 and SSM | 50000 to $5 \times 10^5$ | 10           | 5000       | Figures 1-2           |
| 2      | Algorithm 2 and SSM | 50000         | 10 to 500    | 5000       | Figures 3-4           |
| 3      | Algorithm 2 and SSM | 50000 to $5 \times 10^5$ | 10           | 5000       | Figures 5-6           |
| 4      | Algorithm 2 and SSM | 50000         | 10 to 500    | 5000       | Figures 7-8           |
| 5      | Algorithm 2 and SSM | 50000         | 10           | 5000 to 50000 | Figures 9-10   |

Table 1: Description of five experiments

| Method                              | $p_{k1}$ | $c_k$          | $P_{0k1}$               |
|-------------------------------------|----------|----------------|-------------------------|
| ONU (from Algorithm 2)             | [17]     | $\tilde{c}_k$ | $\frac{1}{2}$           |
| ONMCNR (from Algorithm 3)          | [17]     | $\tilde{c}_k$ | $\frac{\|M_{k(i)}\|_2}{\|N_{k(i)}\|_2}$ |
| OPL (from Algorithm 2)             | [17]     | $\hat{c}_k$   | Null                    |
| ONC (from Algorithm 2)             | [15]     | $\hat{c}_k$   | Null                    |
| UU (from Algorithm 2)              | $\frac{1}{n_k}$ | $\hat{c}_k$ | Null                    |

Table 2: Explanation of sampling methods with different probabilities and block sizes

In the first two experiments, we compare Algorithm 2 and SSM for different $c$ and $K$, respectively. The corresponding numerical results are shown in Figures 1-4. From these figures, we can find that, for Case II, OPL and ONC outperform SSM in accuracy for different $c$ or different $K$, however, they need more computing time. While, the improvement in accuracy is more than the increment in computing time. For Case I, the four methods have similar performances in accuracy, and OPL and ONC are a little expensive. These findings are consistent with the theoretical results of these methods. Furthermore, it is interesting to find that UU may be superior to SSM in accuracy and CPU time for Case II.
Figure 1: Comparison of relative errors for Algorithm 2 and SSM varying with $c$

Figure 2: Comparison of CPU time for Algorithm 2 and SSM varying with $c$
Figure 3: Comparison of relative errors for Algorithm 2 and SSM varying with $K$

Figure 4: Comparison of CPU time for Algorithm 2 and SSM varying with $K$

The third and fourth experiments are utilized to compare Algorithms 2 and 3 for different $c$ and different $K$, respectively. Based on the numerical results presented in Figures 5-8, we get that, for
Case II, OPL always performs best in accuracy and needs most CPU time in most of cases. For different $c$, ONMCNR has the similar performance in accuracy to OPL, however, for large $K$, i.e., small $c_0/K$, it has the worst accuracy. It is a little strange and we have no reasonable explanation at present. In addition, ONC always performs quite well. It needs least CPU time but has the similar accuracy to OPL. For Case I, the four methods perform similarly in accuracy and CPU time.

Figure 5: Comparison of relative errors for Algorithms 2 and 3 varying with $c$
Figure 6: Comparison of CPU time for Algorithms 2 and 3 varying with $c$

Figure 7: Comparison of relative errors for Algorithms 2 and 3 varying with $K$
In the last experiment, we compare Algorithms 2 and 3 for different $c_0$. The corresponding numerical results are shown in Figures 9 and 10. From these figures, it is easy to see that, for Case II, OPL and ONMCNR have the same performances in accuracy for large $c_0$, i.e., large $c_0/K$, and similar performances in CPU time for very large $c_0$. The reason for the latter is that, in this case, the computation complexities of $\|C_0kD_0k\|_F^2$ and $\|M_kN_k\|_F^2$ are similar. In addition, as before, ONC always performs quite well. For Case I, the four methods show the similar accuracy for different $c_0$. 

Figure 8: Comparison of CPU time for Algorithms 2 and 3 varying with $K$.
In a word, for matrices whose rows or columns norms are nonuniform, OPL performs best in accuracy in all cases and worst in CPU time in most cases. When \( c_0/K \) is large, ONMCNR and
OPL have almost the same performances in accuracy and CPU time. In addition, ONC always performs quite well.

5. Concluding Remarks

We present the optimal sampling probabilities and sampling block sizes in the randomized sampling algorithm for block matrix multiplication. Modified sampling block sizes and a two step algorithm for reducing the computation cost are also provided. Numerical experiments show that our new methods outperform the SSM method in [7] in accuracy with a little extra computation cost.

It is easy to see that the blocks of the matrices can be regarded as the single matrices scattered at multiple locations. So, the proposed methods are applicable to distributed data and distributed computations and hence should have many potential important applications in the age of big data.

Appendix A  Proof of Theorem 4

We first deduce that

$$
\sum_{h=1}^{m} \sum_{f=1}^{p} \sigma^2 = \sum_{k=1}^{K} \frac{\|M_k^{(i)}\|_2^2 \|N_k^{(i)}\|_2^2}{c_k p_k} - \sum_{k=1}^{K} \frac{\|M_k N_k\|_F^2}{c_k}
\leq \frac{1}{\beta c} \left( \frac{\theta_2}{\theta_1} \right)^2 \left( \sum_{k=1}^{K} \sum_{i=1}^{n_k} \|M_k^{(i)}\|_2 \|N_k^{(i)}\|_2 \right)^2 - \frac{(1 - \theta_2)}{c} \left( \frac{\theta_1}{\theta_2} \right)^2 \left( \sum_{k=1}^{K} \sum_{i=1}^{n_k} \|M_k^{(i)}\|_2 \|N_k^{(i)}\|_2 \right)^2
\leq \frac{\theta_2 - \theta_1 \beta + \theta_2 \theta_1 \beta}{\beta c (\theta_2 \theta_1)^{1/2}} \|M\|_F^2 \|N\|_F^2
= \frac{\varphi^2}{\beta c} \|M\|_F^2 \|N\|_F^2,
$$

where the second inequality is derived from the Cauchy-Schwarz inequality. To prove (22), we define a event $\theta$ as

$$
\|MN - CD\|_F \leq \frac{\eta}{\sqrt{\beta c}} \|M\|_F \|N\|_F.
$$

Thus, as long as getting $\text{Pr}[\theta] \geq 1 - \delta$, (22) is proved. To explain easily, we define a function

$$
G(x) = \|MN - CD\|_F^2
$$
with random variable \( x = (1(i_1), \ldots, 1(i_n), 2(i_1), \ldots, 2(i_{c_k}), \ldots, K(i_1), \ldots, K(i_{c_k})) \) standing for the positions of sampled results, where \( k(i_t) \) denotes the picked \( t \)-th column (row) from the \( k \)-th block of \( M(N) \), for \( k = 1, \ldots, K \) and \( t = 1, \ldots, c_k \). It is will be shown that changing one coordinate \( k(i_t) \) at a time does not change the value of \( G \) too much. Considering \( x \) and \( x' \) differing only in the \( k(i_t) \)-th coordinate, we can construct corresponding \( \|MN - CD\|_F^2 \) and \( \|MN - C'D'\|_F^2 \), respectively. Note that \( C' \) (\( D' \)) differs from \( C \) (\( D \)) in only a single column (row). So,

\[
\|CD - C'D'\|_F = \frac{\|M^{k(i_t)}N_{k(i_t)}\|_F}{ckp_{k_{i_{t}}}} - \frac{\|M^{k(i_t')N_{k(i_t')}}\|_F}{ckp_{k_{i_{t}'}}}
\]

\[
\leq \frac{1}{ckp_{k_{i_{t}'}}}\|M^{k(i_t)}N_{k(i_t)}\|_F + \frac{1}{ckp_{k_{i_{t}}}}\|M^{k(i_t')}N_{k(i_t')}\|_F
\]

\[
\leq \frac{2}{ck}\|M^{k(i_t)}N_{k(i_t)}\|_F \leq \frac{2}{ck}p_{k_{i_{t}'}}\|MN\|_F\|N\|_F
\]

\[
\leq \frac{2}{\beta c}\left(\frac{\theta_2}{\theta_1}\right)\|MN\|_F\|N\|_F
\]

where \( \frac{\|M^{k(i_t)}N_{k(i_t)}\|_F}{p_{k_{i_{t}'}}} = \max_{i_t=1,\ldots,n_k} \frac{\|M^{k(i_t)}\|_F\|N_{k(i_t)}\|_2}{p_{k_{i_{t}'}}} \). Furthermore, since

\[
\|MN - CD\|_F \leq \|MN - C'D'\|_F + \|CD - C'D'\|_F
\]

\[
\leq \|MN - C'D'\|_F + \frac{2}{\beta c}\left(\frac{\theta_2}{\theta_1}\right)\|MN\|_F\|N\|_F
\]

and

\[
\|MN - C'D'\|_F \leq \|MN - CD\|_F + \|CD - C'D'\|_F
\]

\[
\leq \|MN - CD\|_F + \frac{2}{\beta c}\left(\frac{\theta_2}{\theta_1}\right)\|MN\|_F\|N\|_F
\]

we have \( |G(x) - G(x')| \leq \|CD - C'D'\|_F \). For convenience, let \( \Delta \) denote \( \frac{2}{\beta c}\left(\frac{\theta_2}{\theta_1}\right)\|MN\|_F\|N\|_F \) and \( \gamma = \sqrt{2\log(1/\delta)}\Delta \). Considering Hoeffding-Azuma inequality \[18] \), the probability inequality

\[
\Pr[\|MN - CD\|_F \geq \varphi \sqrt{\beta c}\|MN\|_F\|N\|_F + \gamma] \leq \exp(-\frac{\gamma^2}{2c\Delta^2}) = \delta.
\]

is attained and the theorem follows.

**Remark 6.** Let \( \theta_2 = \theta_1 < 1 \) and \( \beta = 1 \), we have \( \eta = (\theta_2)^2 + \sqrt{8\log(1/\delta)} \) in Theorem 4. It is smaller than the one in [16, Theorem 1], i.e., \( \eta = 1 + \sqrt{8\log(1/\delta)} \). This is because when computing the upper bound of \( \sum_{h=1}^{m}\sum_{f=1}^{1}\sigma^2 \), we do not throw away the second item \( -\sum_{k=1}^{K}\frac{\|M^{k}N_{k}\|_2^2}{n_k} \).
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