Performance Comparison of Accurate Matrix Multiplication

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Introduction

This talk is concerned with accurate matrix multiplication for floating-point matrices.

Floating-point numbers as defined by IEEE 754 has finite information,

- 24 siginificand bits for binary32
- 53 siginificand bits for binary64

Therefore, rounding error may occur in each arithmetic operation.

Notation

- $\mathbb{F}$: the set of floating-point numbers.
- $A \in \mathbb{F}^{m \times n}, B \in \mathbb{F}^{n \times p}$, we compute the matrix multiplication AB.
- $\mathrm{fl}(\cdots)$ means that an expression is evaluated by fl-pt arithmetic.
- $\mathbf{u}$: unit roundoff (binary64: $\mathbf{u} = 2^{-53}$)

For $\mathrm{fl}(\cdots)$, we assume that neither overflow nor underflow occur.

Introduction

Matrix multiplication consists of dot products:

$$c_{ij} = \sum_{k=1}^{n} a_{ik} b_{kj}.$$

For example,

$$a_{11}b_{11} + a_{12}b_{21} + a_{13}b_{31} + \cdots + a_{1n}b_{n1}.$$

Maximally, rounding errors occur $2n - 1$ times.

Introduction

In the worst case, the computed result is inaccurate due to accumulation of rounding errors. From an a priori error analysis, we have the following error bound

$$|\mathrm{fl}(AB) - AB| \le \frac{n\mathbf{u}}{1 - n\mathbf{u}}|A||B|,$$

namely

$$\frac{|\mathrm{fl}(AB) - AB|_{ij}}{|AB|_{ij}} \le \frac{n\mathbf{u}}{1 - n\mathbf{u}}\frac{(|A||B|)_{ij}}{|AB|_{ij}}.$$

Introduction

We develop a new and accurate algorithm for matrix multiplication.

An error bound for a computed result by our algorithm satisfies

$$|AB - \tilde{C}| \le \mathbf{u}|AB|.$$

Overview of our algorithm is

Error-Free Transformation of Matrix Multiplication

+

Accurate Summation Algorithm

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Naive Approach

We apply Veltkamp-Dekker's error-free transformation of a product of floating-point number. For $a, b, x, y \in \mathbb{F}$, their algorithm transforms

$$a * b = x + y, \quad x = \mathrm{fl}(a * b), \quad \mathbf{u}|x| \geq |y|.$$

It requires 17 floating-point operations.

Naive Approach

Applying error-free transformation by Veltkamp and Dekker,

$$(AB)_{ij} = \sum_{k=1}^{n} a_{ik}b_{kj} = a_{i1}b_{1j} + a_{i2}b_{2j} + \cdots + a_{in}b_{nj} = \sum_{k=1}^{2n} v_k.$$

S.M.Rump, T. Ogita, S. Oishi:
Accurate floating-point summation part II: Sign, K-fold faithful and rounding to nearest. Siam J. Sci. Comput., 31(2):1269-1302, 2008.

Then

$$|AB - \tilde{C}| \leq \mathbf{u}|AB|.$$

Accurate Matrix Multiplication

We introduce the error-free transformation of the matrix product. Both A and B are divided into an unevaluated sum of k and l floating-point matrices, respectively, i.e.

$$A = A^{(1)} + A^{(2)} + \cdots + A^{(k)}, \quad B = B^{(1)} + B^{(2)} + \cdots + B^{(l)}$$

and for all k and l

$$A^{(k)} \in \mathbb{F}^{m\times n}, \quad B^{(l)} \in \mathbb{F}^{n\times p}, \quad \mathrm{fl}(A^{(k)}B^{(l)}) = A^{(k)}B^{(l)}.$$

$$q = \texttt{size}(A, 2);$$
$$k = 1;$$
$$\beta = \mathrm{fl}(\lceil(-\log_2(\mathbf{u}) + \log 2(q))/2)\rceil);$$
$$A^{(i)} = \texttt{zeros}(\texttt{size}(A));$$
$$\texttt{while}\ (\texttt{norm}(A, inf)\tilde{}= 0)$$
$$\quad \mu = \max(\texttt{abs}(A), [], 2); \quad \%\ \mu(i) = \max_{1\le j\le q} a_{ij}$$
$$\quad \texttt{if}\ (\max(\mu) == 0),\ \texttt{return};\ \texttt{end}$$
$$\quad w = \mathrm{fl}(2.\hat{}(\texttt{ceil}(\log 2(\mu)) + \beta));$$
$$\quad S = \texttt{repmat}(w, 1, q); \quad \%\ w \cdot e^T$$
$$\quad A^{(k)} = \mathrm{fl}((A + S) - S);$$
$$\quad A = \mathrm{fl}(A - A^{(k)});$$
$$\quad k = k + 1;$$
$$\texttt{end}$$

Accurate Matrix Multiplication

Expanding the expression,

$$AB = (A^{(1)} + A^{(2)} + \cdots + A^{(k)})(B^{(1)} + B^{(2)} + \cdots + B^{(l)}),$$

AB is transformed into

$$AB = \sum_{i=1}^{kl} C^{(i)}, \quad C \in \mathbb{F}^{m \times p}.$$

By using Rump-Ogita-Oishi's NearSum algorithm,

$$|AB - \tilde{C}| \leq \mathbf{u}|AB|.$$

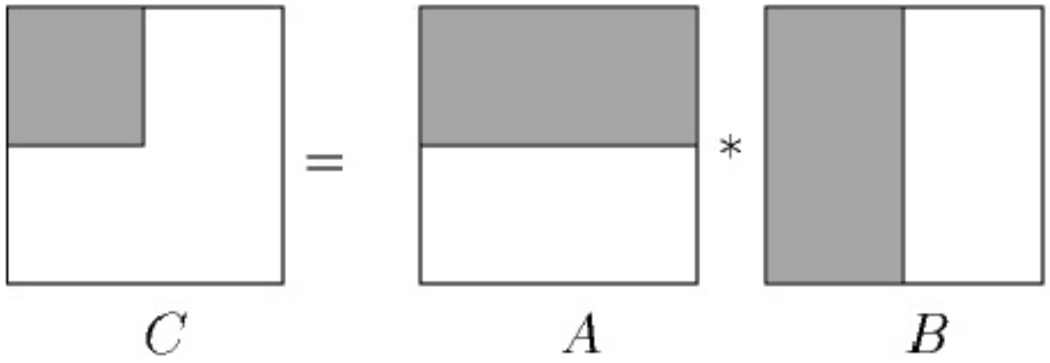
Advantage and Disadvantage

Advantage: Dependence of High Performance Library

Disadvantage: Memory Consumption.

K. Ozaki, T. Ogita, S. Oishi, S. M. Rump: Error-Free Transformation of Matrix Multiplication by Using Fast Routines of Matrix Multiplication and its Applications, Numerical Algorithms, Vol. 59:1 (2012), pp. 95-118.

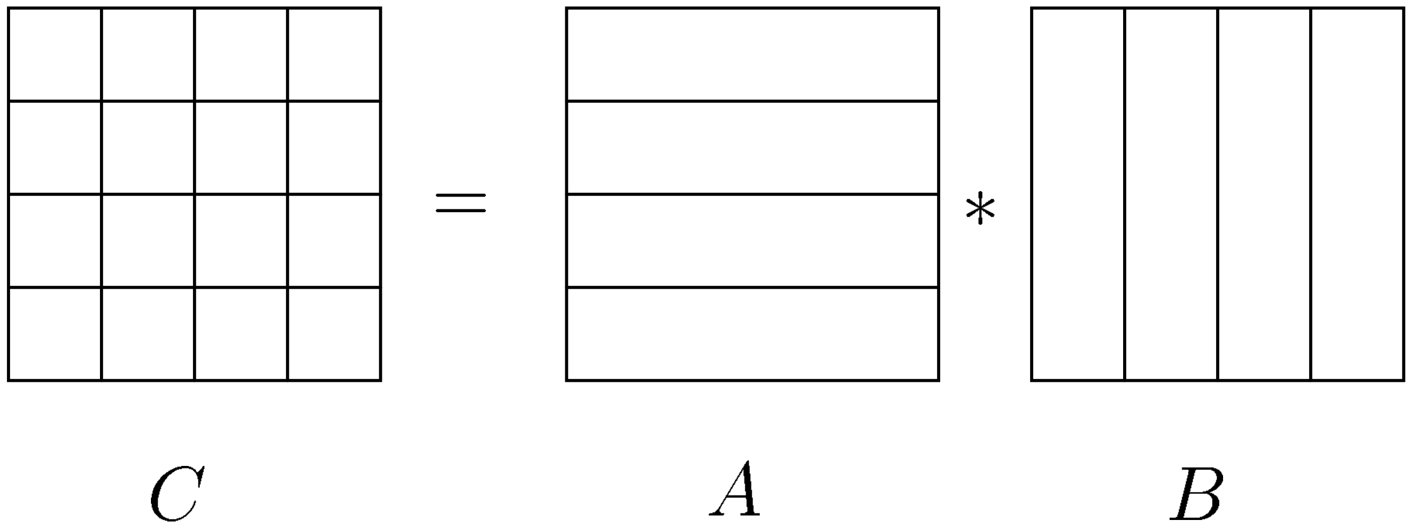
Memory Reduced Implementation



Assume that $A, B \in \mathbb{F}^{n\times n}$ (n is even), and we use MATLAB notation.

$$C(1:n/2, 1:n/2) = A(1:n/2, :) * B(:, 1:n/2)$$

Memory Reduced Implementation



We call this method Type 1.

Memory Reduced Implementation

k : the number of blocks

`accmul` : usual accurate matrix multiplication

```
d = n/k;
for i = 1 : k
  for j = 1 : k
    C((i − 1)d + 1 : i ∗ d, (j − 1)d + 1 : j ∗ d) =
        accmul(A((i − 1)d + 1 : i ∗ d, :)∗
         B(:, (j − 1)d + 1 : j ∗ d));
  end
end
```

Memory Reduced Implementation

Table 1: Comparison of FLOPS (Core i7-2620M, 2.66GHz, 2 cores).

A	B	FLOPS
$\mathbb{F}^{1200\times1200}$	$\mathbb{F}^{1200\times1200}$	36.83
$\mathbb{F}^{600\times1200}$	$\mathbb{F}^{1200\times600}$	32.85
$\mathbb{F}^{300\times1200}$	$\mathbb{F}^{1200\times300}$	30.10
$\mathbb{F}^{2400\times2400}$	$\mathbb{F}^{2400\times2400}$	40.24
$\mathbb{F}^{1200\times2400}$	$\mathbb{F}^{2400\times1200}$	37.98
$\mathbb{F}^{600\times2400}$	$\mathbb{F}^{2400\times600}$	33.17

Memory Reduced Implementation

Table 2: Comparison of FLOPS (Core i7-2620M, 2.66GHz, 2 cores).

A	B	FLOPS
$\mathbb{F}^{4800\times4800}$	$\mathbb{F}^{4800\times4800}$	33.36
$\mathbb{F}^{2400\times4800}$	$\mathbb{F}^{4800\times2400}$	36.72
$\mathbb{F}^{1200\times4800}$	$\mathbb{F}^{4800\times1200}$	36.20
$\mathbb{F}^{9600\times9600}$	$\mathbb{F}^{9600\times9600}$	39.72
$\mathbb{F}^{4800\times9600}$	$\mathbb{F}^{9600\times4800}$	42.02
$\mathbb{F}^{2400\times9600}$	$\mathbb{F}^{9600\times2400}$	41.86

Memory Reduced Implementation

Table 3: Comparison of FLOPS (Xeon X5550, 2.67GHz, 2 CPU, 8 cores).

A	B	FLOPS
$\mathbb{F}^{1200\times1200}$	$\mathbb{F}^{1200\times1200}$	62.2
$\mathbb{F}^{600\times1200}$	$\mathbb{F}^{1200\times600}$	48.2
$\mathbb{F}^{300\times1200}$	$\mathbb{F}^{1200\times300}$	32.3
$\mathbb{F}^{2400\times2400}$	$\mathbb{F}^{2400\times2400}$	75.1
$\mathbb{F}^{1200\times2400}$	$\mathbb{F}^{2400\times1200}$	70.7
$\mathbb{F}^{600\times2400}$	$\mathbb{F}^{2400\times600}$	66.5

Memory Reduced Implementation

Table 4: Comparison of FLOPS (Xeon X5550, 2.67GHz, 2 CPU, 8 cores).

A	B	FLOPS
$\mathbb{F}^{4800\times 4800}$	$\mathbb{F}^{4800\times 4800}$	77.4
$\mathbb{F}^{2400\times 4800}$	$\mathbb{F}^{4800\times 2400}$	77.4
$\mathbb{F}^{1200\times 4800}$	$\mathbb{F}^{4800\times 1200}$	74.1
$\mathbb{F}^{9600\times 9600}$	$\mathbb{F}^{9600\times 9600}$	77.4
$\mathbb{F}^{4800\times 9600}$	$\mathbb{F}^{9600\times 4800}$	75.1
$\mathbb{F}^{2400\times 9600}$	$\mathbb{F}^{9600\times 2400}$	77.7

Memory Reduced Implementation

Next, we consider an another way (Type 2).

$$
\begin{array}{rrl}
A^{(1)} + \underline{A}^{(2)}, & B^{(1)} + \underline{B}^{(2)} \Longrightarrow & A^{(1)}B^{(1)} \\
A^{(1)} + \underline{A}^{(2)}, & \cancel{B^{(1)}} + B^{(2)} + \underline{B}^{(3)} \Longrightarrow & A^{(1)}B^{(2)} \\
A^{(1)} + \underline{A}^{(2)}, & \cancel{B^{(2)}} + B^{(3)} + \underline{B}^{(4)} \Longrightarrow & A^{(1)}B^{(3)} \\
 & \vdots & \\
\cancel{A^{(1)}} + A^{(2)} + \underline{A}^{(3)}, & B^{(1)} + \underline{B}^{(2)} \Longrightarrow & A^{(2)}B^{(1)} \\
\cancel{A^{(1)}} + A^{(2)} + \underline{A}^{(3)}, & \cancel{B^{(1)}} + B^{(2)} + \underline{B}^{(3)} \Longrightarrow & A^{(2)}B^{(2)}
\end{array}
$$

Let μ be space for n-by-n matrix. Pure implementation requires

$$(n_A + n_B + n_A n_B)\mu.$$

Type 1 with k blocks requires

$$(n_A + n_B)\mu/k + n_A n_B \mu/k^2$$

Type 2 requires

$$4\mu + n_A n_B \mu$$

Combination fo Type 1 and Type 2 requires

$$4\mu/k + n_A n_B \mu/k^2.$$

Memory Reduced Implementation

Let $A(1 : n/2, :)$ be A_1.

If A is divided into

$$A = A^{(1)} + A^{(2)} + A^{(3)} + A^{(4)}.$$

The following may happen:

$$A_1 = A_1^{(1)} + A_1^{(2)} + A_1^{(3)}.$$

The number of matrix products may be reduced by block computations.

Numerical Results

We compare computing times for

- M1: Naive Approach for rounding to nearest.
- M2 ($k = 1$): EFT + rounding to nearest
- M2 ($k > 1$): EFT + rounding to nearest with block computations

Computational environments:
Core i7-2620M, MATLAB2011b, Intel C++ Compiler 12.0.

Numerical Results

Table 5: Comparison of computing times and ratio.

Method \ n	1200	2400	4800
M1	15.8 (131.3)	136.1 (194.4)	1362 (203.6)
M2 (k=1)	1.58 (13.1)	17.0 (24.3)	132.0 (19.7)
M2 (k=2)	1.76 (14.6)	17.8 (25.5)	132.9 (19.8)
M2 (k=3)	1.76 (14.6)	18.4 (26.4)	135.0 (20.1)
M2 (k=4)	1.74 (14.3)	19.2 (27.4)	139.7 (20.8)
M2 (k=5)	1.80 (14.9)	19.8 (28.3)	142.0 (21.2)

A and B are generated as `randn`(n).

Numerical Results

Table 6: Comparison of ratio with various ϕ ($n = 1200$).

Method \ ϕ	0	1	4	7	10
M1	149.6	146.7	134.7	143.3	81.1
M2 (k=1)	16.1	17.2	29.7	46.0	42.1
M2 (k=2)	17.5	19.7	31.3	49.8	43.8
M2 (k=4)	17.7	18.7	30.9	57.5	47.4

A and B are generated as $(\mathrm{rand}(n) - 0.5).*\exp(\phi * \mathrm{randn}(n))$.
If ϕ is large, there is big difference in the order of magnitude.

Numerical Results

Table 7: Comparison of ratio with various ϕ ($n = 2400$).

Method \ ϕ	0	1	4	7	10
M1	171.1	170.3	174.4	171.3	169.0
M2 (k=1)	16.2	19.3	34.3	54.9	84.2
M2 (k=2)	16.9	18.5	35.5	55.4	85.1
M2 (k=4)	17.6	19.6	39.6	61.0	92.3

A and B are generated as $(\mathrm{rand}(n) - 0.5). * \exp(\phi * \mathrm{randn}(n))$.
If ϕ is large, there is big difference in the order of magnitude.

Numerical Results

Table 8: Comparison of ratio with various ϕ ($n = 4800$).

Method \ ϕ	0	1	4	7	10
M1	204.5	170.3	204.7	203.8	205.9
M2 (k=1)	15.3	18.7	32.6	70.1	169.3
M2 (k=2)	15.6	19.2	33.3	59.4	89.4
M2 (k=4)	16.2	19.9	34.2	61.6	92.7

A and B are generated as $(\mathrm{rand}(n) - 0.5). * \exp(\phi * \mathrm{randn}(n))$.
If ϕ is large, there is big difference in the order of magnitude.

Conclusion

- EFT of matrix multiplication efficiently helps accurate computing in terms of computational performance
- Block computations reduce the amount of working memory.
- Block computations don't significantly slow computational performance down (sometimes work faster than original one).

Thank you very much for your kind attention!