Practicality of Large Scale Fast Matrix Multiplication

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Classical matrix multiplication is nearly ubiquitous, even though asymptotically faster algorithms have been known since 1969.

Concerns about fast matrix multiplication:

- Practical speed
- Stability

This talk addresses both concerns.
Outline

- Strassen’s algorithm
- New parallel algorithm
  - Communication optimal
  - Faster in practice
- Stability of Strassen
  - Normwise error bound
  - Diagonal scaling, improved error bounds
  - Stability experiments
Recall: Strassen’s fast matrix multiplication

Strassen’s original algorithm uses 7 multiplies and 18 adds for $n = 2$. It is applied recursively (blockwise).

\[
\begin{align*}
M_1 &= (A_{11} + A_{22}) \cdot (B_{11} + B_{22}) \\
M_2 &= (A_{21} + A_{22}) \cdot B_{11} \\
M_3 &= A_{11} \cdot (B_{12} - B_{22}) \\
M_4 &= A_{22} \cdot (B_{21} - B_{11}) \\
M_5 &= (A_{11} + A_{12}) \cdot B_{22} \\
M_6 &= (A_{21} - A_{11}) \cdot (B_{11} + B_{12}) \\
M_7 &= (A_{12} - A_{22}) \cdot (B_{21} + B_{22}) \\
C_{11} &= M_1 + M_4 - M_5 + M_7 \\
C_{12} &= M_3 + M_5 \\
C_{21} &= M_2 + M_4 \\
C_{22} &= M_1 - M_2 + M_3 + M_6
\end{align*}
\]

\[T(n) = 7 \cdot T(n/2) + O(n^2)\]

Improved by Winograd to 15 additions
Two kinds of costs:

- Arithmetic (FLOPs)
- Communication: moving data between
  - levels of a memory hierarchy (sequential case)
  - over a network connecting processors (parallel case)

Communication is becoming more expensive relative to computation
Communication lower bounds for matrix multiplication

Strassen:

\[ \Omega \left( \left( \frac{n}{\sqrt{M}} \right)^{\log_2 7} M \right) \]

Classic (cubic):

\[ \Omega \left( \left( \frac{n}{\sqrt{M}} \right)^{\log_2 8} M \right) \]
Communication lower bounds for matrix multiplication

Algorithms attaining these bounds?

Strassen: \( \Omega \left( \left( \frac{n}{\sqrt{M}} \right)^{\log_2 7} M \right) \)

Classic (cubic): \( \Omega \left( \left( \frac{n}{\sqrt{M}} \right)^{\log_2 8} M \right) \)

Sequential

Distributed

Distributed

Benjamin Lipshitz

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Communication lower bounds for matrix multiplication

Algorithms attaining these bounds?

Strassen:

\[ \Omega \left( \left( \frac{n}{\sqrt{M}} \right)^{\log_2 7} M \right) \]

Classic (cubic):

\[ \Omega \left( \left( \frac{n}{\sqrt{M}} \right)^{\log_2 8} M \right) \]

\[ \Omega \left( \left( \frac{n^2}{P^2 / \log_2 7} \right) \right) \]

\[ \Omega \left( \left( \frac{n^2}{P^2 / \log_2 8} \right) \right) \]
Lessons from lower bounds

- Don’t use a classical algorithm for the communication
  - Strassen can communicate less than classical
- Make local multiplies as large as possible
- Use all available memory, up to $O(n^2/P^2/\log_2^7)$
  - Communication bound decreases with increased memory
- Send memory size messages to minimize latency
Main Idea of CAPS algorithm

At each level of recursion tree, choose either breadth-first or depth-first traversal of the recursion tree

**Breadth-First-Search (BFS)**

- Runs all 7 multiplies in parallel
  - each uses \( P/7 \) processors
- Requires 7/4 as much extra memory
- Requires communication, but
- All BFS minimizes communication if possible

**Depth-First-Search (DFS)**

- Runs all 7 multiplies sequentially
  - each uses all \( P \) processors
- Requires 1/4 as much extra memory
- No immediate communication
- Increases bandwidth by factor of 7/4
- Increases latency by factor of 7
Main Idea of CAPS algorithm

At each level of recursion tree, choose either breadth-first or depth-first traversal of the recursion tree

**Breadth-First-Search (BFS)**

**Depth-First-Search (DFS)**

```
CAPS
if enough memory and P \geq 7
then BFS step
else DFS step
end if
```
## Asymptotic costs analysis

<table>
<thead>
<tr>
<th></th>
<th><strong>Flops</strong></th>
<th><strong>Bandwidth</strong></th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Strassen</strong></td>
<td><strong>Lower Bound</strong></td>
<td><strong>2D-Strassen</strong></td>
</tr>
<tr>
<td></td>
<td>$\frac{n^{\omega_0}}{P}$</td>
<td>$\frac{n^{\omega_0}}{P^{(\omega_0-1)/2}}$</td>
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<tr>
<td></td>
<td>$\max \left{ \frac{n^{\omega_0}}{PM^{\omega_0/2-1}}, \frac{n^2}{P^{2/\omega_0}} \right}$</td>
<td>$\frac{n^2}{P^{1/2}}$</td>
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<tr>
<td></td>
<td><strong>Strassen-2D</strong></td>
<td></td>
</tr>
<tr>
<td></td>
<td>$\frac{(7/8)^\ell n^3}{P}$</td>
<td></td>
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</tbody>
</table>
Performance of CAPS

Strong-scaling on Franklin (Cray XT4), $n = 94080$.

24%-184% faster than previous Strassen-based algorithms
51%-84% faster than best classical algorithm
The CAPS matrix multiplication algorithm

- is communication optimal
  - matches the communication lower bounds
  - moves asymptotically less data than all existing algorithms

- is faster: asymptotically and in practice
  - faster than any parallel classical algorithm can be
  - faster than any parallel Strassen-based algorithm we are aware of

- applies to other fast matrix multiplication algorithms
  - but there might not be any other practical ones
Stability

- CAPS has the same stability properties as any other Strassen (Strassen-Winograd) algorithm.

- Weaker stability guarantee than classical, but still norm-wise stable.

- This can be improved through diagonal scaling.
  - Two best scaling schemes give incomparable bounds
  - Can check which bound is better in $O(n^2)$ time

- The improved error bounds match those of matrix factorization such as classical LU and QR.
Diagonal Scaling

Outside scaling: $D^A C D^B = (D^A A)(B D^B)$
- Scale so each row of $A$ and each column of $B$ has unit norm.
- Explicitly:
  - Let $D^A_{ii} = (\|A(i,:)\|)^{-1}$, and $D^B_{jj} = (\|B(:,j)\|)^{-1}$.
  - Scale $A' = D^A A$, and $B' = B D^B$.
  - Use Strassen for the product $C' = A' B'$.
  - Unscale $C = (D^A)^{-1} C' (D^B)^{-1}$.
Diagonal Scaling

Outside scaling: $D^A C D^B = (D^A A)(B D^B)$

- Scale so each row of $A$ and each column of $B$ has unit norm.
- Explicitly:
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  - Use Strassen for the product $C' = A' B'$.
  - Unsacle $C = (D^A)^{-1} C' (D^B)^{-1}$.

Inside scaling: $C = (A D)(D^{-1} B)$

- Scale so each column of $A$ has the same norm as the corresponding row of $B$.
- Explicitly:
  - Let $D_{ii} = (\|A(:,i)\|/\|B(i,:)\|)^{-1/2}$.
  - Scale $A' = AD$, and $B' = D^{-1} B$.
  - Use Strassen for the product $C = A' B'$.
Error bounds

\[ |C_{ij} - \hat{C}_{ij}| \leq O(\epsilon)f(n) \cdot \ldots \]

Classical:
\[ (|A| \cdot |B|)_{ij} \]

Outside-Inside:
\[ \|A(i,:)\|\|B(:,j)\|\|D^A A \cdot BD^B \| \]

Inside-Outside:
\[ \|(AD)(i,:)\|\|(D^{-1}B)(:)\| \]

Outside:
\[ \|A(i,:)\|\|B(:,j)\| \]

Inside:
\[ \|A \cdot |B|\| \]

No Scaling:
\[ \|A\|\|B\| \]

X \rightarrow Y means that bound X is stronger than bound Y.
Scaling example: easy case

\[
\max_{i,j} \left| \frac{\hat{C}_{ij} - C_{ij}}{|A| \cdot |B|_{ij}} \right|
\]

\[
\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix}
\]

\( n = 1024 \)
Scaling example: needs outer scaling

\[
\frac{\hat{C}_{ij} - C_{ij}}{|A| \cdot |B|}_{ij}
\]

\[
\max_{ij} \left| \frac{\hat{C}_{ij} - C_{ij}}{|A| \cdot |B|}_{ij} \right|
\]

\[
\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} \epsilon & 1 \\ \epsilon & 1 \end{pmatrix}
\]

\[
n = 1024
\]
Scaling example: needs inner and outer

\[
\max_{ij} \left| \hat{C}_{ij} - C_{ij} \right| \frac{1}{(|A| \cdot |B|)_{ij}}
\]

\[
egin{pmatrix}
1 & \epsilon \\
\epsilon & \epsilon
\end{pmatrix} \cdot \begin{pmatrix}
\epsilon & 1 \\
1 & \epsilon^{-1}
\end{pmatrix}
\]

\(n = 1024\)
Scaling example: inner-outer better than outer-inner

\[ \max_{ij} \left| \hat{C}_{ij} - C_{ij} \right| \left/ \left( |A| \cdot |B| \right)_{ij} \right. \]

\[ \begin{pmatrix} \epsilon & \epsilon \\ 1 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & \epsilon^{-1} \\ 1 & 1 \end{pmatrix} \]

\( n = 1024 \)
Scaling example: outer-inner better than inner-outer

\[
\max_{ij} \left| \hat{C}_{ij} - C_{ij} \right| \frac{1}{\max \{|A|, |B|\}}
\]

\[
\begin{pmatrix}
1 & \epsilon^{-1} \\
1 & 1
\end{pmatrix}
\begin{pmatrix}
\epsilon & 1 \\
\epsilon & 1
\end{pmatrix}
\]

\(n = 1024\)
Scaling example: problems scaling can’t fix

\[
\frac{|\tilde{C}_{ij} - C_{ij}|}{|A| \cdot |B|}_{ij}
\]

\[
\max_{ij} \left( \begin{array}{cc}
1 & \epsilon^{-1} \\
1 & 1
\end{array} \right) \cdot \left( \begin{array}{cc}
1 & \epsilon^{-1} \\
1 & 1
\end{array} \right)
\]

\[n = 1024\]
Error bounds

\[ |C_{ij} - \hat{C}_{ij}| \leq O(\epsilon)f(n) \cdot \ldots \]

Classical:
\((|A| \cdot |B|)_{ij}\)

Outside-Inside:
\[ \|A(i,:)\| \|B(:,j)\| \|D^A A \cdot BD^B\| \]

Inside-Outside:
\[ \|(AD)(i,:)\| \|(D^{-1}B)(:,j)\| \]

Outside:
\[ \|A(i,:)\| \|B(:,j)\| \]

Inside:
\[ \||A| \cdot |B|| \]

No Scaling:
\[ \|A\| \|B\| \]

\(X \rightarrow Y\) means that bound \(X\) is stronger than bound \(Y\).
Stability summary

- Scaling improves error bound of Strassen
  - To be comparable to many other algorithms
  - But still not as good as classical algorithm
- Applies to other fast matrix multiplication algorithms
- Inner-then-outer or outer-then-inner scaling are best
- Can choose between them by evaluating their bounds
- Open problem: simultaneously attain inner and outer scaling bounds?
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Thank You!

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Communication-optimal parallel algorithm for Strassen's matrix multiplication.
To appear in SPAA 2012.

Strong scaling of matrix multiplication algorithms and memory-independent communication lower bounds.
To appear in SPAA 2012.

Graph expansion and communication costs of fast matrix multiplication.

B. Lipshitz, G. Ballard, O. Schwartz, and J. Demmel.
Submitted to SC 2012.
Extra slides

1. Previous Parallel Strassen
2. Data Layout
3. Strassen-Winograd Algorithm
4. Hardware scaling
5. Time breakdown
6. Small problems
Previous parallel Strassen-based algorithms

2D-Strassen: [Luo, Drake 95]

- Run classical 2D inter-processors.
  - Same communication costs as classical 2D.
- Run Strassen locally.
  - Can’t use Strassen on the full matrix size.
Previous parallel Strassen-based algorithms

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Strassen-2D: [Luo, Drake 95; Grayson, Shah, van de Geijn 95]
- Run Strassen inter-processors
  - This part can be done without communication.
- Then run classical 2D.
  - Communication costs grow exponentially with the number of Strassen steps.
Previous parallel Strassen-based algorithms

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- Run Strassen inter-processors
  - This part can be done without communication.
- Then run classical 2D.
  - Communication costs grow exponentially with the number of Strassen steps.

Neither is communication optimal
Data Layout
Strassen-Winograd Algorithm

\[
\left( \begin{array}{c|c} C_{11} & C_{12} \\ \hline C_{21} & C_{22} \end{array} \right) = C = A \cdot B = \left( \begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array} \right) \cdot \left( \begin{array}{c|c} A_{11} & A_{12} \\ \hline A_{21} & A_{22} \end{array} \right)
\]

\[
S_0 = A_{11} \quad T_0 = B_{11} \quad Q_i = S_i \cdot T_i
\]
\[
S_1 = A_{12} \quad T_1 = B_{21} \quad U_1 = Q_i + Q_4
\]
\[
S_2 = A_{21} + A_{22} \quad T_2 = B_{12} + B_{11} \quad U_2 = U_1 + Q_5
\]
\[
S_3 = S_2 - A_{12} \quad T_3 = B_{22} - T_2 \quad U_3 = U_1 + Q_5
\]
\[
S_4 = A_{11} - A_{21} \quad T_4 = B_{22} - B_{12} \quad C_{11} = Q_1 + Q_2
\]
\[
S_5 = A_{12} + S_3 \quad T_5 = B_{22} \quad C_{12} = U_3 + Q_6
\]
\[
S_6 = A_{22} \quad T_6 = T_3 - B_{21} \quad C_{21} = U_2 - Q_7
\]
\[
C_{22} = U_2 + Q_3
\]
Implications for hardware scaling

Requirements so that dense matrix multiplication is computation bound.

<table>
<thead>
<tr>
<th></th>
<th>Bandwidth Requirement</th>
<th>Latency Requirement</th>
</tr>
</thead>
<tbody>
<tr>
<td>Classic</td>
<td>$\gamma M^{1/2} \geq \beta$</td>
<td>$\gamma M^{3/2} \geq \alpha$</td>
</tr>
<tr>
<td>Strassen</td>
<td>$\gamma M^{\omega_0/2-1} \geq \beta$</td>
<td>$\gamma M^{\omega_0/2} \geq \alpha$</td>
</tr>
</tbody>
</table>

Strassen performs fewer flops and less communication, but is more demanding on the hardware.
CAPS time breakdown

$n = 94080$ on Franklin

Wall time (seconds)

- strong scaling range
- local multiplications
- communication
- local additions
- re-arrangement
- other
- perfect scaling

Extras
Performance on small problems

$n = 3136$ on Franklin

![Graph showing execution time vs. number of cores]
Sequential recursive Strassen is communication optimal

- Run Strassen algorithm recursively.
- When blocks are small enough, work in localy memory, so no further bandwidth cost

\[ W(n, M) = \begin{cases} 
7W\left(\frac{n}{2}, M\right) + O(n^2) & \text{if } 3n^2 > M \\
O(n^2) & \text{otherwise}
\end{cases} \]

- Solution is

\[ W(n, M) = O\left(\frac{n^{\omega_0}}{M^{\omega_0/2-1}}\right) \]
Extra slides

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