Cache Friendly Sparse Matrix Vector Multilication

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Plan

1. Cache Complexity
2. Locality Issues in Sparse Matrix Vector Multiplication
3. Binary Reflected Gray Codes
4. Cache Complexity Analyzes
5. Experimentation
Once upon a time everything was slow in a computer.

The CPU-Memory Gap

The increasing gap between DRAM, disk, and CPU speeds.
But I/O complexity was already there

STOC(Milwaukee 1981), 326-333.

I/O COMPLEXITY: THE RED-BLUE PEBBLE GAME

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In this paper, the red-blue pebble game is proposed to model the input-output complexity of algorithms. Using the pebble game formulation, a number of lower bound results for the I/O requirement are proven. For example, it is shown that to perform the n-point FFT or the ordinary nxn matrix multiplication algorithm with O(S) memory, at least \( \Omega(n \log n/\log S) \) or \( \Omega(n^3/\sqrt{S}) \), respectively, time is needed for the I/O. Similar results are obtained for algorithms for several other problems. All of the lower bounds presented are the best possible in the sense that they are achievable by certain decomposition schemes. The paper is organized according to the techniques used to derive these lower bounds.

In Section 2 we formally define the pebble game and point out its relation to the I/O problem. In Section 3 we show that lower bounds for I/O in the pebble game can be established by studying the so-called S-partitioning problem. This is the key result of the paper in the sense that it provides the basis for the derivation of all the lower bounds. In Section 4 we prove a lower bound for the FFT algorithm. Lower bounds in Section 5 are based on the information speed function, which
**Abstract** This paper presents asymptotically optimal algorithms for rectangular matrix transpose, FFT, and sorting on computers with multiple levels of caching. Unlike previous optimal algorithms, these algorithms are *cache oblivious*: no variables dependent on hardware parameters, such as cache size and cache-line length, need to be tuned to achieve optimality. Nevertheless, these algorithms use an optimal amount of work and move data optimally among multiple levels of cache. For a cache with size $Z$ and cache-line length $L$ where $Z = \Omega(L^2)$ the number of cache misses for an $m \times n$ matrix transpose is $\Theta(1 + mn/L)$. The number of cache misses for either an $n$-point FFT or the sorting of $n$ numbers is $\Theta(1 + (n/L)(1 + \log_Z n))$. We also give an $\Theta(mnp)$-work algorithm to multiply an $m \times n$ matrix by an $n \times p$ matrix that is organized by an optimal replacement strategy.

**Cache-Oblivious Algorithms**

**EXTENDED ABSTRACT**

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Figure 1: The ideal-cache model
The \((Z, L)\) ideal cache model

- The ideal cache is **fully associative**: cache lines can be stored anywhere in the cache.
- The ideal cache uses the **optimal off-line strategy of replacing** the cache line whose next access is furthest in the future, and thus it exploits temporal locality perfectly.

**Figure 1**: The ideal-cache model
Plan

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An illustrative example (1/2)

Input matrix and vector

\[
A = \begin{pmatrix}
a_{0,0} & 0 & 0 & 0 & a_{0,4} & 0 \\
0 & 0 & a_{1,2} & 0 & 0 & a_{1,5} \\
0 & a_{2,1} & 0 & a_{2,3} & 0 & 0
\end{pmatrix}
\times
\begin{pmatrix}
x_0 \\
x_1 \\
x_2 \\
x_3 \\
x_4 \\
x_5
\end{pmatrix}
\]

Cache misses due to \(x\)

Assume that the cache has 2 lines each of 2 words. Assume also that the cache is dedicated to store the entries from \(x\):

\[
\begin{bmatrix}
\emptyset & \emptyset \\
\emptyset & \emptyset
\end{bmatrix}
\begin{bmatrix}
x_0 & x_1 \\
x_4 & x_5
\end{bmatrix}
\begin{bmatrix}
x_0 & x_1 \\
x_2 & x_3
\end{bmatrix}
\begin{bmatrix}
x_4 & x_5 \\
x_0 & x_1
\end{bmatrix}
\]
An illustrative example (2/2)

After reordering the columns of $A$

$$A' = \begin{pmatrix} a_{0,0} & a_{0,4} & 0 & 0 & 0 & 0 \\ 0 & 0 & a_{1,2} & a_{1,5} & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & a_{2,1} & a_{2,3} \end{pmatrix} \times \begin{pmatrix} x' \\ x_0 \\ x_4 \\ x_2 \\ x_5 \\ x_1 \\ x_3 \end{pmatrix}$$

Cache misses due to $x'$

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Plan

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Gray Codes

Definition

- For $N = 2^n$, an $n$-bit code $C_n = (u_1, u_2, \ldots, u_N)$, where $N = 2^n$, is a Gray code if $u_i$ and $u_{i+1}$ differ in exactly one bit, for all $i$.
- This corresponds to a Hamiltonian path (cycle) in the $n$-dimensional hypercube.

Binary Reflected Gray Codes

The reflected Gray code $\Gamma^n$ is defined recursively by

$$
\Gamma^1 = (0, 1) \text{ and } \Gamma^{n+1} = 0 \Gamma^n, 1 \Gamma^n R
$$

Introduced by Frank Gray 1953 for shaft encoders

$$
\Gamma^3 = 000, 001, 011, 010, 110, 111, 101, 100.
$$
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$$\Gamma^3 = 000, 001, 011, 010, 110, 111, 101, 100.$$
Gray Codes

Binary reflected Gray code for arithmetic operations

- Integers of dimension $m$ can be represented by a data structure that uses $m + \log m + O(\log\log m)$ bits so that increment and decrement operations require at most $\log m + O(\log\log m)$ bit inspections and 6 bit changes per operation. (M.Z. Rahman and J.I. Munro, 2007).
- They have also good results for addition and subtraction.

Binary reflected Gray code for sorting big integers

- A set of $n$ binary strings of dimension $m$ is sparse if any 2 strings are very unlikely to have two consecutive 1’s at the same positions.
- BRGC-Sorting a sparse set of $n$ binary strings of dimension $m$ requires
  - $O(\tau)$ index comparisons and $O(\tau + n)$ data-structure updates,
  - where $\tau$ is the total number of 1’s.
  (Sardar Anisul Haque and M.M.M., 2010).
- Thus, BRGC-sorting a sparse set of $n$ big integers fits within $O(\tau + n)$. 

(Haque, Hossain, Moreno Maza)
Gray Codes

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(Haque, Hossain, Moreno Maza)
Binary Reflected Gray Codes

From the University of Florida sparse matrix collection

(Haque, Hossain, Moreno Maza)
Non-zero streams
Plan

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Cache complexity estimates

Expected cache misses in accessing $x$ when $A$ is random

Recall that $A$ is very sparse. Assume that $n$ is large enough such that the vector $x$ does not fit into the cache, typically $n \in O(Z^2)$

$$Q_1 = \frac{Z}{L} + (\tau - \frac{Z}{L}) \frac{n - \frac{Z}{L}}{n}.$$ 

Indeed, no spatial locality should be expected in accessing $x$.

Expected cache misses in accessing $x$ after BRGC-reordering $A$

$$Q_2 = \frac{n}{L} + \frac{Z}{L} + (n - \frac{Z}{L}) \frac{n/\rho - \frac{Z}{L}}{n/\rho} + (\tau - 2n) \frac{cn/\rho - \frac{Z}{L}}{cn/\rho},$$

where $c$ is the average number of nonzero streams under one step of first level nonzero stream and $1 \leq c \leq \rho$. 

(Haque, Hossain, Moreno Maza)
Cache complexity estimates

Expected cache misses in accessing $x$ when $A$ is **random**
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Expected cache misses in accessing $x$ after **BRGC-reordering** $A$

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where $c$ is the average number of nonzero streams under one step of first level nonzero stream and $1 \leq c \leq \rho$. 
How much do we save?

For our large test matrices and today’s L2 cache sizes, the following conditions hold:

- $n \in O(Z^2)$ and
- $Z > 2^{10}$.

Using MAPLE, we could prove the following relation:

$$Q_1 - Q_2 \approx n.$$
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## Experimentation

<table>
<thead>
<tr>
<th>Matrix name</th>
<th>m</th>
<th>n</th>
<th>$\tau$</th>
<th>SPM\times V with BRGC ordering</th>
<th>SPM\times V without any ordering</th>
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</tbody>
</table>
Summary

1. Reordering columns or rows in SPMxV can improve locality significantly.
2. Optimal reordering is computationally hard.
3. Preprocessing cost needs to be amortized against the SPMXVs in the conjugate gradient type algorithms.
4. BRGC ordering improves locality.
5. BRGC ordering technique can be implemented in linear time w.r.t. $\tau$.
6. The cost of BRGC ordering can be amortized before $\sqrt{n}$ SPMXVs in conjugate Gradient type algorithms.
7. The matrices used in our experimentation are very sparse but already have nice structures, so they are far from the (ideal) random case.