CS 598: Communication Cost Analysis of Algorithms

Lecture 9: The Ideal Cache Model and the Discrete Fourier Transform

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Algorithmic cache management

Consider a computer with unlimited memory and a cache of size H

- we can design algorithms by manually managing cache transfers
- simple metrics:
  - amount of data moved from memory to cache (bandwidth cost)
  - number of synchronous memory-to-cache transfers (latency cost)
- generally, efficient algorithms in this model try to select blocks of computation that minimize the surface-to-volume ratio
  - i.e., do as much computation with the cache-resident data as possible
  - in other words, exploit temporal and spatial locality

Cache-efficient matrix multiplication

Consider multiplication of $n \times n$ matrices $C = A \cdot B$

For $i \in [1, n/s], j \in [1, n/t]$, $k \in [1, n/v]$, define blocks $C[i, j]$, $A[i, k]$, $B[k, j]$ with dimensions $s \times t$, $s \times v$, and $v \times t$, respectively

```
for (i = 1 to n/s)
  for (j = 1 to n/t)
    initialize C[i,j] = 0 in cache
    for (k = 1 to n/v)
      load A[i,k] into cache
      load B[k,j] into cache
      C[i,j] = C[i,j] + A[i,k]*B[k,j]
    end
    write C[i,j] to memory
  end
end
```

Q: What restriction must we impose to insure $A[i, k]$, $B[k, j]$ and $C[i, j]$ fit in cache simultaneously?

A: $st + sv + vt \leq H$

Memory-bandwidth analysis of matrix multiplication

So we have the constraint, $st + sv + vt \leq H$

- there are a total of $(n/s)(n/t)(n/v)$ inner loop iterations
- Q: what is the asymptotic memory latency cost of the algorithm
- A: the number of inner loop iterations, $n^3/(stv)$
- since each block of C stays resident in the innermost loop, we write each element of C to memory only once
- we read each block $s \times v$ block of A and $v \times t$ block of B in each innermost loop
- Q: how many times do we read each element of A and B?
- A: n/t and n/s, respectively
- therefore, the bandwidth cost is $Q = n^2 + (n/s + n/t)n^2 = n^2 + n^3/s + n^3/t$
- if we pick $s = t = v = \sqrt{H/3}$, we satisfy the constraint and obtain $Q \approx 2n^3/\sqrt{H/3}$, with $n^3/H^{3/2}$ memory latency cost
- if we pick $s = t = \sqrt{H - 2\sqrt{H}}$ and $v = 1$, we obtain $Q \approx 2n^3/\sqrt{H}$ with n^3/H memory latency cost

Memory-bandwidth cost of LU decomposition

For most dense linear algebra problems, achieving good bandwidth cost is strictly easier in the sequential case than in the parallel case

- example: non-pivoted LU factorization
- we can use the same recursive algorithm, two recursive calls, $O(1)$ matrix multiplications
- $T(n, H) = 2T(n/2) + O(\nu \cdot n^3/\sqrt{H})$ where ν is inverse of memory bandwidth
- cost decreases geometrically by factor of 4 with each level, we can stop at base case dimension $n_0 = \sqrt{H}$ and compute LU sequentially
- memory latency cost is just $O(n^3/H^{3/2} \cdot \nu)$, same as matrix multiplication
- Q: given memory bandwidth cost $O(n^3/\sqrt{H} \cdot \nu)$, why is it not possible to have less than a $\Theta(n^3/H^{3/2})$ memory latency cost?
- A: we cannot transfer messages larger than the cache size H

Memory-bandwidth cost of eigenvalue decompositions

The symmetric matrix eigenvalue problem (nearly same as nonsymmtric SVD) provides a nice example of where memory-bandwidth requires extra consideration with respect to distributed memory bandwidth cost

- probably the last dense numerical linear algebra problem we study in this course
- given a symmetric matrix A, we would like to compute its eigenvalues
- stable algorithms work by first reducing A to tridiagonal form, then using the MRRR algorithm
- the reduction to tridiagonal form dominates the cost
- needs to be done via two-sided orthogonalization to preserve eigenvalues $T = Q^T AQ$

Direct tridiagonalization

We can perform two-sided orthogonalization via Householder QR

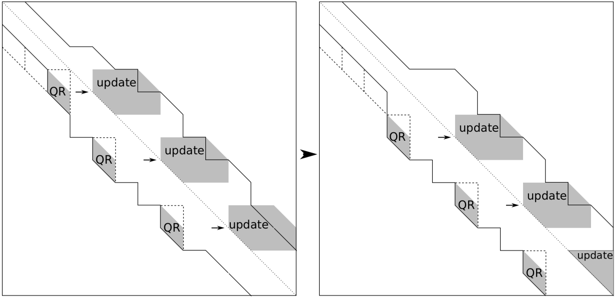
- compute Householder vector to eliminate $n-2$ lower entries of first column
- $Q_1^T A = (I - 2uu^T)A$ does not affect top row, so we can perform $Q_1^T A Q_1$
- applying Q_1^T from the left is independent across columns
- applying Q_1 from the right is independent across rows
- this means we need to compute $Q_1^T A Q_1$ fully, before we can compute the Householder vector of the next column
- for designing a 2D algorithm, we can keep A in place and broadcast the vectors, for $O(n^2/\sqrt{P})$ communication
- but if the matrix blocks do not fit in cache ($n^2/P \geq H$), we will have $O(n^3/P)$ memory bandwidth cost (no reuse), rather than $O(n^3/(P\sqrt{H}))$

Full-to-band reduction

We can alleviate the problem by reducing to a banded matrix first

- compute rectangular QR of $n - b \times b$ lower left minor (submatrix)
- $Q_1^T A = (I - 2uu^T)A$ reduces first b columns to bandwidth $2b$ and does not affect top b rows, so we can perform $Q_1^T A Q_1$
- now we can perform the trailing matrix update by matrix multiplication with rectangular matrices of dimensions $(n - b) \times b$
- Q: what is the minimal b we would want to pick to get $\sqrt{H}$ reuse of trailing matrix entries, and consequently $O(n^3/(P\sqrt{H}))$ memory bandwidth cost?
- A: $b = \sqrt{H}$
- it then remains to reduce the banded matrix to tridiagonal form, which can be done via bulge chasing [Lang 1993]

Symmetric band reduction (bulge chasing)



Ideal cache model

A more accurate model is to consider a cache line size L in addition to the cache size H

- each memory-to-cache transfer has size L
- new unified metric: cache misses (number of cache lines transferred)
- the bandwidth cost is the number of cache misses multiplied by L
- the (old) latency cost (number of transfers) is disregarded
- assume 'tall' cache, $L \leq \sqrt{H}$ (more convenient, $H = \Omega(L^2)$)
- we can now consider different caching protocols
- an ideal cache model corresponds to the assumption that the protocol always makes the best decision
- this ideal cache model is in a sense equivalent to a manually orchestrated cache protocol
- arbitrary manual orchestration can be achieved with an LRU (lest-recently-used protocol)

Matrix transposition in the ideal cache model

Matrix multiplication bandwidth cost with a tall cache is not affected by L

- if we read square blocks into cache they have dimension $\Theta(L)$
- if we compute outer products, just need to transpose B initially
- $n \times n$ matrix transposition becomes non-trivial
  - when $L = 1$ (original model), there is no notion of how a matrix is laid out in memory
  - for general L, we should read $\sqrt{H} \times \sqrt{H}$ blocks into cache, transpose them, then write them to memory to get linear bandwidth cost $O(n^2)$
  - matrix transposition is a very useful subroutine when we need to ensure contiguous access to cache lines

Cache obliviousness

Introduced by Frigo, Leiserson, Prokop, Ramachadran (original paper worth reading)

- basic idea: algorithms should not be parameterized by architectural parameters
- good ideas in computer science are most often good abstractions
- designing an algorithm obliviously of cache size makes it portable and efficient for all levels of a cache hierarchy
- cache oblivious algorithms are stated without explicit control of data movement
- their communication cost is derived by assuming an ideal cache model
- ideal caches can be simulated by an LRU cache protocol for most (regular) algorithms

Cache oblivious matrix transposition

Given $m \times n$ matrix A, compute $B = A^T$

- if $m \leq n$ subdivide $A = [A_1 \ A_2]$ and $B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}$ and compute recursively, $B_1 = A_1^T$, $B_2 = A_2^T$
- if $m > n$ subdivide $A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$ and $B = [B_1 \ B_2]$ and compute recursively, $B_1 = A_1^T$, $B_2 = A_2^T$

obtains linear bandwidth cost $T(mn) = 2T(mn/2)$, $T(1) = O(1)$, so $T(mn) = O(mn)$

Cache oblivious matrix multiplication

Given $m \times k$ matrix A and $k \times n$ matrix B, compute $m \times n$ matrix $C = AB$

- if $k \geq m$ and $k \geq m$ subdivide $A = \begin{bmatrix} A_1 & A_2 \end{bmatrix}$ and $B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}$ and compute recursively, $\bar{C} = A_1 B_1$, $\hat{C} = A_2 B_2$, then $C = \bar{C} + \hat{C}$
- if $n > k$ and $n \geq m$ subdivide $C = \begin{bmatrix} C_1 & C_2 \end{bmatrix}$ and $B = \begin{bmatrix} B_1 & B_2 \end{bmatrix}$ and compute recursively, $C_1 = AB_1$, $C_2 = AB_2$
- if $m > k$ and $m > n$ subdivide $C = \begin{bmatrix} C_1 \\ C_2 \end{bmatrix}$ and $A = \begin{bmatrix} A_1 \\ A_2 \end{bmatrix}$ and compute recursively, $C_1 = A_1 B$, $C_2 = A_2 B$

Short pause

DFT matrix

These notes are based on James Demmel's book, "Applied Numerical Linear Algebra"

For any n, let $\omega_n = e^{-2\pi i/n}$, so $\omega_n^{n/2} = -1$ and $\omega_n^n = 1$, a DFT matrix of dimension n is given by

$$\forall j, k \in [0, n-1] \quad D_n(j,k) = \omega_n^{jk}$$

for example

$$D_4 = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & \omega & \omega^2 & \omega^3 \\ 1 & \omega^2 & \omega^4 & \omega^6 \\ 1 & \omega^3 & \omega^6 & \omega^9 \end{bmatrix}$$

DFT matrix

The matrix $A = \frac{1}{\sqrt{n}} D_n$ is symmetric and unitary $A = A^T = A^*$, $AA^{-1} = I$

D_n^{-1} has the form $D_n^{-1}(j,k) = (1/n)\omega^{-jk}$, now $X = D_n D_n^{-1}$ has the form

$$X(j,k) = (1/n)\sum_{l=0}^{n-1} \omega_n^{jl}\omega_n^{-lk} = (1/n)\sum_{l=0}^{n-1} \omega_n^{l(j-k)}$$

Clearly $X(j,j) = 1$, while $X(j,j+t) = (1/n)\sum_{l=0}^{n-1}(\omega_n^t)^l$ is a geometric sum for $t \neq 0$, so

$$X(j,j+t) = (1/n)\frac{1-\omega^{nt}}{1-\omega^t} = 0 \quad \text{since} \quad 1-\omega^{nt} = 1-(\omega^n)^t = 1-1^t = 0$$

Convolution

A convolution takes as input vectors a and b and computes vector c

$$\forall k \in [0, n-1] \quad c(k) = \sum_{j=0}^{k} a(j)b(k-j)$$

- given coefficients of two polynomials of degree $n/2$ stored in a and b, the convolution computes the coefficients c of the product of the two polynomials
- naive evaluation costs $O(n^2)$ operations
- the convolution can also be interpreted as matrix-vector multiplication with a triangular Toeplitz matrix

$$[c(0)\ c(1)\ c(2)\ c(3)] = [a(0)\ a(1)\ a(2)\ a(3)] \cdot \begin{bmatrix} b(0) & b(1) & b(2) & b(3) \\ 0 & b(0) & b(1) & b(2) \\ 0 & 0 & b(0) & b(1) \\ 0 & 0 & 0 & b(0) \end{bmatrix}$$

Convolution via DFT

We can compute

$$\forall k \in [0, n-1] \quad c(k) = \sum_{j=0}^{k} a(j)b(k-j)$$

via $c = D_n^{-1}[(D_n a) \odot (D_n b)]$ where $\odot$ is an elementwise product

$$z = v \odot w \rightarrow z(i) = v(i) \cdot w(i)$$

- we can find some intuition for this by thinking back to polynomial multiplication
- the DFT $D_n a$ evaluates a polynomial $f(x)$ at $x = \omega^j$ for $j \in [0, n-1]$
- the elementwise product computes the values of the polynomial product at these points
- the inverse DFT D_n^{-1} interpolates back from the points to get the coefficients of the polynomial product

Convolution via DFT

The polynomial interpretation is abstract, lets see what happens algebraically

- first lets write out the full expression in indexed form

$$\begin{aligned} c(k) &= \sum_s D_n^{-1}(k,s)\Big(\sum_j D_n(s,j)a(j)\Big)\Big(\sum_t D_n(s,t)b(t)\Big) \\ &= \sum_s \omega_n^{-ks}\Big(\sum_j \omega_n^{sj} a(j)\Big)\Big(\sum_t \omega_n^{st} b(t)\Big) \end{aligned}$$

- now, lets rearrange the order of the summations to see what happens to every product of a and b

$$\begin{aligned} c(k) &= \sum_s \sum_j \sum_t \omega_n^{-ks}\omega_n^{sj}\omega_n^{st} a(j)b(t) \\ &= \sum_s \sum_j \sum_t \omega_n^{(j+t-k)s} a(j)b(t) \end{aligned}$$

- we can observe that when $j+t-k=0$ the products $\omega_n^{(s+t-j)k}=1$, so the terms $a(j)b(k-j)$ survive!
- For any $u=j+t-k\neq 0$, we observe $\sum_s (\omega_n^u)^s=0$, as for $D_nD_n^{-1}$