Homework and Schedule

Second homework (matrix product with asymptotic performance):

- Consider only the square case: A, B and C are of size $N \times N$
- You can assume that N is a multiple of $\sqrt{M} - 1$

NB: Homeworks will be graded (they replace exams) and have to be done by yourself. Similar works will get a 0.

Next week:

- Wednesday course moved to 10h15
- Exchange with CR13: "Approximation Theory and Proof Assistants: Certified Computations"

Part 2: External Memory and Cache Oblivious Algorithms

CR05: Data Aware Algorithms

September 16, 2020

Outline

Ideal Cache Model

Properties of real cache:

- Memory/cache divided into blocks (or lines or pages) of size B
- When requested data not in cache (cache miss), corresponding block automatically loaded
- Limited associativity:
  - each block of memory belongs to a cluster (usually computed as *address* % M)
  - at most c blocks of a cluster can be stored in cache at once (c-way associative)
  - Trade-off between hit rate and time for searching the cache
- If cache full, blocks have to be evicted: Standard block replacement policy: LRU (also LFU or FIFO)

Ideal cache model:

- Fully associative
  $c = \infty$, blocks can be store everywhere in the cache
- Optimal replacement policy
  Belady's rule:
- Tall cache: $M/B \gg B$ $\quad (M = \Theta(B^2))$

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LRU vs. Optimal Replacement Policy

replacement policy	cache size	nb of cache misses
LRU	k_{LRU}	$T_{LRU}(s)$
OPT	$k_{\text{OPT}} \leq k_{\text{LRU}}$	$T_{OPT}(s)$

OPT: optimal (offline) replacement policy (Belady's rule)

Theorem (Sleator and Tarjan, 1985).

For any sequence s:

$$T_{\text{LRU}}(s) \leq \frac{k_{\text{LRU}}}{k_{\text{LRU}} - k_{\text{OPT}} + 1} T_{\text{OPT}}(s) + k_{\text{OPT}}$$

- Also true for FIFO or LFU (minor adaptation in the proof)
- If LRU cache initially contains all pages in OPT cache: remove the additive term

Theorem (Bound on competitive ratio).

Assume there exists a and b such that $T_A(s) \leq aT_{\text{OPT}}(s) + b$ for all s, then $a \geq k_A/(k_A - k_{\text{OPT}} + 1)$.

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LRU competitive ratio – Proof

- Consider any subsequence t of s, such that $C_{\mathsf{LRU}}(t) \leq k_{\mathsf{LRU}}$ (t should not include first request)
- Let p_i be the block request right before t in s
- If LRU loads twice the same block in s, then $C_{\mathsf{LRU}}(t) \geq k_{\mathsf{LRU}} + 1$ (contradiction)
- Same if LRU loads p_i during t
- Thus on t, LRU loads $C_{\mathsf{LRU}}(t)$ different blocks, different from p_i
- When starting t, OPT has p_i in cache
- On t, OPT must load at least $C_{\mathsf{LRU}}(t) - k_{\mathsf{OPT}} + 1$

- Partition s into $s_0, s_1, \ldots, s_n$ such that $C_{\mathsf{LRU}}(s_0) \leq k_{\mathsf{LRU}}$ and $C_{\mathsf{LRU}}(s_i) = k_{\mathsf{LRU}}$ for $i > 1$
- On s_0, $C_{\mathsf{OPT}}(s_0) \geq C_{\mathsf{LRU}}(s_0) - k_{\mathsf{OPT}}$
- In total for LRU: $C_{\mathsf{LRU}} = C_{\mathsf{LRU}}(s_0) + nk_{\mathsf{LRU}}$
- In total for OPT: $C_{\mathsf{OPT}} \geq C_{\mathsf{LRU}}(s_0) - k_{\mathsf{OPT}} + n(k_{\mathsf{LRU}} - k_{\mathsf{OPT}} + 1)$

Bound on Competitive Ratio – Proof

- Let S_A^{init} (resp. $S_{\text{OPT}}^{\text{init}}$) the set of blocks initially in A'cache (resp. OPT's cache)
- Consider the block request sequence made of two steps:

  S_1: $k_A - k_{\text{OPT}} + 1$ (new) blocks not in $S_A^{\text{init}} \cup S_{\text{OPT}}^{\text{init}}$
  S_2: $k_{\text{OPT}} - 1$ blocks s.t. then next block is always in $(S_{\text{OPT}}^{\text{init}} \cup S_1) \backslash S_A$

  NB: step 2 is possible since $|S_{\text{OPT}}^{\text{init}} \cup S_1| = k_A + 1$

- A loads one block for each request of both steps: k_A loads
- OPT loads one block only in S_1: $k_A - k_{\text{OPT}} + 1$ loads

NB: Repeat this process to create arbitrarily long sequences.

Justification of the Ideal Cache Model

Theorem (Frigo et al, 1999).

If an algorithm makes T memory transfers with a cache of size $M/2$ with optimal replacement, then it makes at most $2T$ transfers with cache size M with LRU.

Definition (Regularity condition).

Let $T(M)$ be the number of memory transfers for an algorithm with cache of size M and an optimal replacement policy. The regularity condition of the algorithm writes

$$T(M) = O(T(M/2))$$

Corollary

If an algorithm follows the regularity condition and makes $T(M)$ transfers with cache size M and an optimal replacement policy, it makes $\Theta(T(M))$ memory transfers with LRU.

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External Memory Model

Model:

- External Memory (or disk): storage
- Internal Memory (or cache): for computations, size M
- Ideal cache model for transfers: blocks of size B
- Input size: N
- Lower-case letters: in number of blocks
  $n = N/B$, $m = M/B$

Theorem.

Scanning N elements stored in a contiguous segment of memory costs at most $\lceil N/B \rceil + 1$ memory transfers.

Outline

Merge Sort in External Memory

Standard Merge Sort: Divide and Conquer

1. Recursively split the array (size N) in two, until reaching size 1
2. Merge two sorted arrays of size L into one of size $2L$ requires $2L$ comparisons

In total: $\log N$ levels, N comparisons in each level

Adaptation for External Memory: Phase 1

- Partition the array in N/M chunks of size M
- Sort each chunks independently ($\rightarrow$ runs)
- Block transfers: $2M/B$ per chunk, $2N/B$ in total
- Number of comparisons: $M \log M$ per chunk, $N \log M$ in total

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Two-Way Merge in External Memory

Phase 2:

Merge two runs R and S of size $L \rightarrow$ one run T of size $2L$

1. Load first blocks $\widehat{R}$ (and $\widehat{S}$) of R (and S)
2. Allocate first block $\widehat{T}$ of T
3. While R and S both not exhausted
   (a) Merge as much $\widehat{R}$ and $\widehat{S}$ into $\widehat{T}$ as possible
   (b) If $\widehat{R}$ (or $\widehat{S}$) gets empty, load new block of R (or S)
   (c) If $\widehat{T}$ gets full, flush it into T
4. Transfer remaining items of R (or S) in T

- Internal memory usage: 3 blocks
- Block transfers: $2L/B$ reads $+$ $2L/B$ writes $= 4L/B$
- Number of comparisons: $2L$

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Total complexity of Two-Way Merge Sort

Analysis at each level:

- At level k: runs of size $2^k M$ (nb: $N/(2^k M)$)
- Merge to reach levels $k = 1 \dots \log_2 N/M$
- Block transfers at level k: $2^{k+1}M/B \times N/(2^k M) = 2N/B$
- Number of comparisons: N

Total complexity of phases 1+2:

- Block transfers: $2N/B(1 + \log_2 N/B) = O(N/B \log_2 N/B)$
- Number of comparisons: $N \log M + N \log_2 N/M = N \log N$

- Internal memory used ?

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- Internal memory used ? only 3 blocks ☹

Optimization: K-Way Merge Sort

- Consider K input runs at each merge step
- Efficient merging, e.g.: MinHeap data structure
  insert, extract: $O(\log K)$
- Complexity of merging K runs of length L: $KL \log K$
- Block transfers: no change ($2KL/B$)

Total complexity of merging:

- Block transfers: $\log_K N/M$ steps $\rightarrow 2N/B \log_K N/M$
- Computations: $N \log K$ per step $\rightarrow N \log K \times \log_K N/M$
  $= N \log_2 N/M$ (id.)

Maximize K to reduce transfers:

- $(K+1)B = M$ (K input blocks $+$ 1 output block)
- Block transfers: $O\left(\frac{N}{B} \log_{\frac{M}{B}} \frac{N}{M}\right)$
- NB: $\log_{M/B} N/M = \log_{M/B} N/B - 1$
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Outline

Lower Bound on Sorting

Theorem.

Sorting N elements in external memory requires $\Theta\left(\frac{N}{B} \log_{\frac{M}{B}} \frac{N}{B}\right)$ block transfers.

Corollary: K-Way Merge Sort is asymptotically optimal

Lower Bound on Sorting – Proof (1/2)

- Comparison based model:
  elements compared when in internal memory
- Inputs of new blocks give new information (but not outputs)
- S_t: number of permutations consistent with knowledge after reading t blocks of inputs
- At the beginning: $S_0 = N!$ possible orderings (no information)
- After reading one block: new information (answer)
  how the elements read are ordered among themselves and among the M elements in memory ?
- Assume X possible answers after one read, then

$$S_{t+1} \geq S_t / X$$

  - Partition of the S_t orderings into X parts
  - There exists a part of size at least S_t/X, that is an answer with at least S_t/X compatible orderings

Lower Bound on Sorting – Proof (2/2)

Bound the number of possible orderings:

(i) When reading a block already seen: $X = \binom{M}{B}$

(ii) When reading a new block (never seen): $X = \binom{M}{B} B!$

NB: at most N/B new blocks (case (i))

From $S_0 = N!$ and $S_{t+1} \geq S_t / X$, we get:

$$S_t \geq \frac{N!}{\binom{M}{B}^t (B!)^{N/B}}$$

$S_t = 1$ for final step

Stirling's formula gives: $\log x! \approx x \log x$ and $\log \binom{x}{y} \approx y \log x/y$ (when $y \ll x$)

$$t = \Omega\left(\frac{N}{B} \log_{\frac{M}{B}} \frac{N}{B}\right)$$

Outline

Permuting

Inputs:

- N elements together with their final position:
  (a,3) (b,2) (c,1) (d,4) $\rightarrow$ c,b,a,d

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Two simple strategies:

- Place each element at its final position, one after the other
  I/O cost: $\Theta(N)$ (cmp cost: $O(N)$)
- Sort elements based on final position
  I/O cost: $\Theta(SORT(N)) = \Theta(N/B \log_{M/B} N/B)$
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Lower-bound:

- Using similar argument, one may prove that the I/O complexity is bounded by $\Theta(\min(SORT(N), N))$
- NB: generally, $SORT(N) \ll N$

Outline

B-Trees

- Problem: Search for a particular element in a huge dataset
- Solution: Search tree with large degree ($\approx B$)

Definition (B-tree with minimum degree d).

Search tree such that:

- Each node (except the root) has at least d children
- Each node has at most $2d - 1$ children
- Node with k children has $k - 1$ keys separating the children
- All leaves have the same depth

Proposed by Bayer and McCreigh (1972)

Search and Insertion in B-Trees

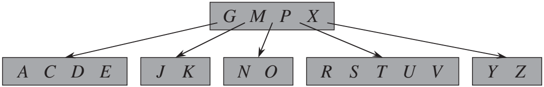
Usually, we require that $d = O(B)$

Lemma.

Searching in a B-Tree requires $O(\log_d N)$ I/Os.

Recursive algorithm for insertion of new key:

1. If root node of current subtree is full ($2d$ children), split it:
   (a) Find median key, send it to the father f
       (if any, otherwise it becomes the new root)
   (b) Keys and subtrees $<$ median key $\rightarrow$ new left subtree of f
   (c) Keys and subtrees $>$ median key $\rightarrow$ new right subtree f
2. If root node of current subtree $=$ leaf, insert new key
3. Otherwise, find correct subtree s, insert recursively in s



NB: height changes only when root is split $\rightarrow$ balanced tree

Number of transfers: $O(h)$

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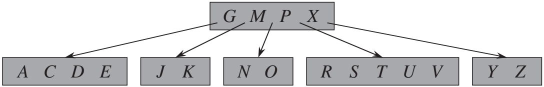

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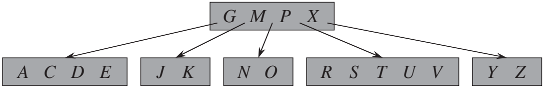

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Suppression in B-Trees

Suppression algorithm of k from a tree with at least d keys:

- If tree=leaf, straightforward
- If $k =$ key of root node:
  - If subtree s immediately left of k has $\geq d$ keys, remove maximum element k' of s, replace k by k'
  - Same on right subtree (with minimum element)
  - Otherwise (both neighbor subtrees have $d-1$ keys): remove k and merge these neighbor subtrees
- If k is in a subtree s, suppress recursively in s
- If T has only $d-1$ keys:
  - Try to steal one key from a neighbor of T with at least d keys
  - Otherwise merge T with one of its neighbors

Number of block transfers: $O(h)$

Usage of B-Trees

Widely used in large database and filesystems
(SQL, ext4, Apple File System, NTFS)

Variants:

- B+ Trees: store data only on leaves
  increase degree $\rightarrow$ reduce height
  add pointer from leaf to next one to speedup sequential access
- B* Trees: better balance of internal node
  (max size: $2b \rightarrow 3b/2$, nodes at least $2/3$ full)
  - When 2 siblings full: split into 3 nodes
  - Pospone splitting: shift keys to neighbors if possible

Searching Lower Bound

Theorem.

Searching for an element among N elements in external memory requires $\Theta(\log_{B+1} N)$ block transfers.

Proof:

- Adversary argument
- Total order of N elements known to the algorithm
- Let C_t be the number of candidates after t reads ($C_0 = N$)
- When a block of size B is read, the $C_t - B$ remaining elements are distributed into $B + 1$ parts, one of them has at least $(C_t - B)/(B + 1)$ elements.
- By induction, $C_t \geq N/(B + 1)^t - (B + 1)/B$

If memory initially full, $C_0 = (N - M)/(M + 1)$, lower bound: $\Theta(\log_{B+1} N/M)$

Outline

Matrix-Matrix Multiplication

The I/O bound on matrix multiplication seen previously is extended:

Theorem.

The number of block transfers for multiplying two $N \times N$ matrices is $\Theta(N^3/(B\sqrt{M}))$ when $M < N^2$.

Blocked algorithms naturally reduces block transfers.

Summary: External Memory Bounds

	Internal Memory (computational complexity)	External Memory (I/O complexity)
Scanning	N	N/B
Sorting	$N \log_2 N$	$N/B \log_{M/B} N/B$
Permuting	N	$\min(N, N/B \log_{M/B} N/B)$
Searching	$\log_2 N$	$\log_B N$
Matrix Mult.	N^3	$N^3/(B\sqrt{M})$

Notes:

- Linear I/O: $O(N/B)$
- Permuting is not linear
- B is an important factor: $\frac{N}{B} < \frac{N}{B} \log_{\frac{M}{B}} \frac{N}{B} \ll N$
- Search tree cannot lead to optimal sort