Algorithms and Datastructures

Cache Efficiency, Divide and Conquer

Prof. Dr. Rolf Backofen

Bioinformatics Group / Department of Computer Science

Algorithms and Datastructures, March 2018

Structure

Cache Efficiency

Introduction

Background:

- Up to now we always counted number of operations
- Assuming this is a good measure for the runtime of a algorithm/tool
- Today we will see examples where this is not suitable

Example:

- We sum up all elements of a field a of size n in ...
  - natural order:

$$\mathrm{sum}(a) = a[1] + a[2] + \cdots + a[n]$$

  - random order:

$$\mathrm{sum}(a) = a[21] + a[5] + \cdots + a[8]$$

Python:

```python
def init(size):
    # use system time as seed
    random.seed(None)

    # set linear order as accessor
    order = [a for a in range(0, size)]

    # init array with random data
    data = [random.random() for a in order]

    return (order, data)
```

Cache Efficiency

Linear Order - Python

Python:

```python
def run(param):
    # unpack data
    (order, data) = param

    # init the sum value
    s = 0

    for index in order:
        s += data[index]

    return s
```

Cache Efficiency

Linear Order

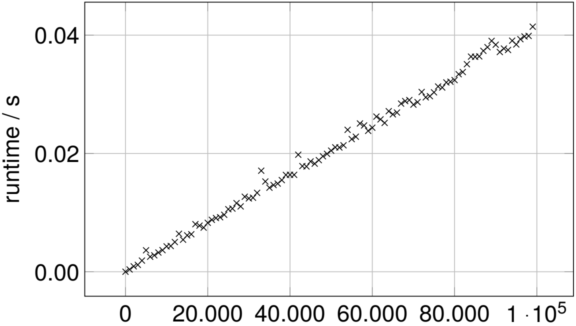


Figure: Summing elements in linear order

Cache Efficiency

Random Order - Python

Python:

```
def init(size):
    # use system time as seed
    random.seed(None)

    # set random order as accessor
    order = [a for a in range(0, size)]
    random.shuffle(order)

    # init array with random data
    data = [random.random() for a in order]

    return (order, data)
```

Cache Efficiency
Random Order

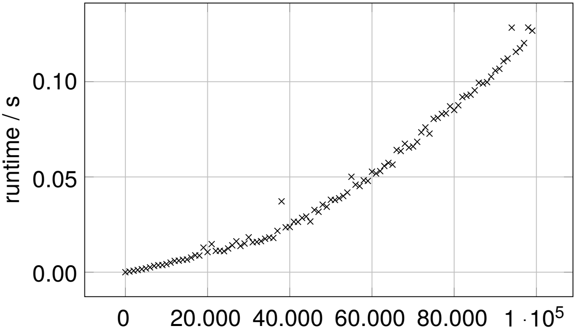


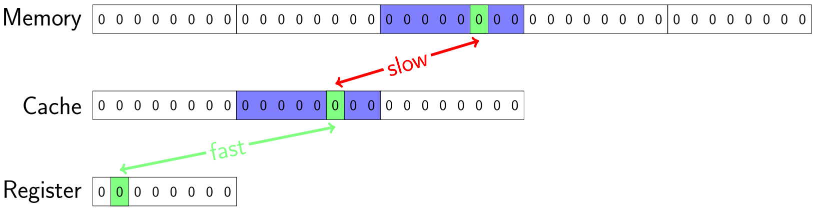
Figure: Summing elements in random order

Conclusion:

- The number of operations are identical for both algorithms
- Accessing elements in random order takes a lot longer (Factor 10)
  Why?
- The costs in terms of memory access are very different

Cache Efficiency

CPU Cache

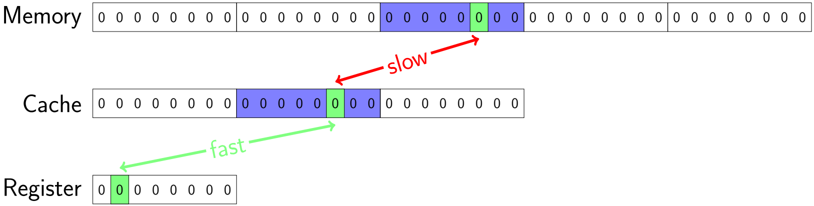


Principle / organization:

- Accessing one byte of the main memory takes $\approx 100\,\text{ns}$
- Accessing one byte of (L1-)cache takes $\approx 1\,\text{ns}$
- Accessing one or more byte/s of main memory loads a whole block $\approx 100\,\text{B}$ into the cache
- As long as this block is in the cache, it is not neccessary to access the memory for bytes of this block

Cache Efficiency

CPU Cache

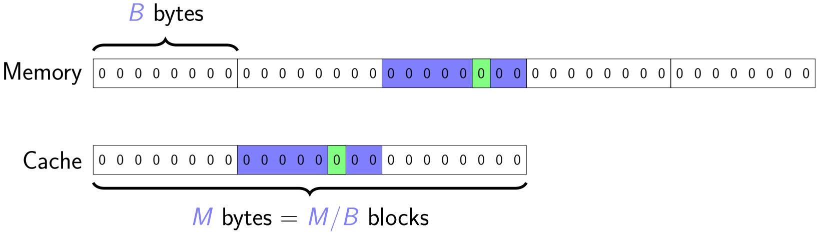


Cache organization:

- The (L1-)cache can hold multiple memory blocks (cache lines)
    - $\approx 100\,\mathrm{kB}$
- If the capacity is reached unused blocks are discarded
    - Least recently used (LRU)
    - Least frequently used (LFU)
    - First in first out (FIFO)
- Details of discarding are not the topic for today

Cache Efficiency

Block Operations

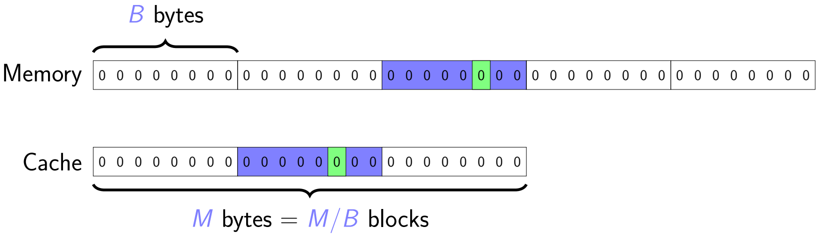


Terminology:

- The system consists of slow and fast memory
- The slow memory is divided in blocks of size B
- The fast cache has size M an can store M/B blocks
- If data is not in fast memory, the corresponding block is loaded into the cache

Cache Efficiency

Block Operations



Terminology:

- The program defines which blocks are held in the cache
- We use the number of block operations as runtime estimation
- We ignore runtime costs of cache accesses / management

Cache Efficiency

Block Operations

Figure: Comparison good / bad locality

Accessing the cache B times:

- Best case: 1 block operation $\rightarrow$ good locality
- Worst case: B block operations $\rightarrow$ bad locality

Cache Efficiency

Block Operations

Additional factors:

- The following settings change only a small constant factor in number of block operations
  - The partionining of the slow memory into blocks
  - If the block is 1 Bytes or 4 Bytes or 8 Bytes

Note:

- If the input size is smaller than M we load the complete data chunk directly into the cache
- Cache handling is only interesting when the input size is greater than M

Cache Efficiency

Block Operations

Typical values: (`Intel©` `i7-4770` Haswell, `WD©` `Blue` 2 TB)

- CPU L1 Cache: $B = 64\,\mathrm{B}$, $M = 4 \times (32\,\mathrm{kB} + 32\,\mathrm{kB})$
- CPU L2 Cache: $B = 64\,\mathrm{B}$, $M = 4 \times 256\,\mathrm{kB}$
- CPU L3 Cache: $B = 64\,\mathrm{B}$, $M = 8\,\mathrm{MB}$
- Disk Cache: $B = 64\,\mathrm{kB}$, $M = 64\,\mathrm{MB}$
  - Many operating systems use free system memory as disk cache

Cache Efficiency
Block Operations

Terminology:

- Block loads on CPU-cache are called cache misses
- Block operations on disk-cache are called IOs (input / output operations)
- These also fall under the term cache efficiency or IO efficiency

Cache Efficiency

Block Operations - Linear Order

Example 1 - Linear order:

- We sum up all elements in natural order

$$\mathrm{sum}(a) = a[1] + a[2] + \cdots + a[n]$$

- The number of block operations is $\mathrm{ceil}\left(\frac{n}{B}\right)$

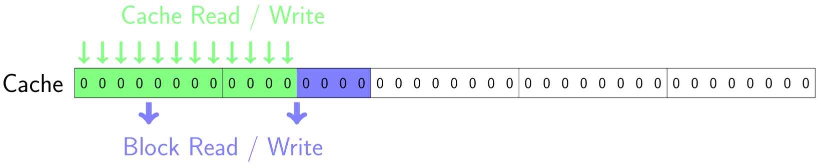


Figure: Good locality of sum operation

Cache Efficiency

Block Operations - Random Order

Example 2 - Random order:

- We sum up all elements in random order

$$\mathrm{sum}(a) = a[21] + a[5] + \cdots + a[8]$$

- The number of block operations is n in the worst case
- This leads to a runtime factor difference of B

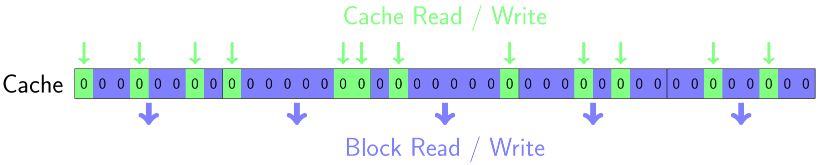


Figure: Bad locality of sum operation

Cache Efficiency

Block Operations

Generally the factor is substantially $< B$

- Even with a random or5bder we access per element 4 (`int`) / neighboring bytes at once
- If not $n \gg M$ the next element might already with a high probability loaded in cache

Cache Efficiency

Block Operations - QuickSort

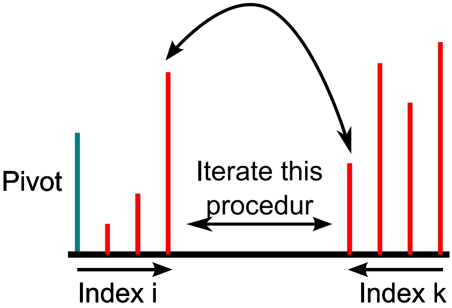
QuickSort:

- **Strategy:** Divide and conquer
- Divide the data into two parts where the “left” part contains all values $\leq$ those in the right part
- Choose one element (e.g the first one) as “pivot”-element
- Ideally both parts are the same size
- Both parts are sorted recursively

Figure: *QuickSort* with pivot-element

Idea of Quicksort

- **at start:** pivot in first position, first re-arrange list such that left part contains small, right part larger elements
- do required changes *in place*



- **end point:** k is left to left-most element greater than pivot

  swap position 0 (pivot) with k (smaller than pivot)

Cache Efficiency

Block Operations - QuickSort - Python

Python:

```python
def quicksort(l, start, end):
  if (end - start) < 1:
    return

  i = start
  k = end
  piv = l[0]

  ...
```

Cache Efficiency

Block Operations - QuickSort - Python

```python
def quicksort(l, start, end):
    ...

    while k > i:
        while l[i] <= piv and i <= end and k > i:
            i += 1
        while l[k] > piv and k >= start and k >= i:
            k -= 1

        if k > i: # swap elements
            (l[i], l[k]) = (l[k], l[i])

    (l[start], l[k]) = (l[k], l[start])
    quicksort(l, start, k - 1)
    quicksort(l, k + 1, end)
```

Cache Efficiency

Block Operations - QuickSort

Number of operations for Quicksort:

- Let $T(n)$ be the runtime for the input size n
- Assumptions:
  - Fields are always separated perfectly in the middle
  - n is a power of two and recursion depth is $k = \log_2 n$

Cache Efficiency

Block Operations - QuickSort

$$
\begin{aligned}
T(n) \quad &\leq \quad \underbrace{A \cdot n}_{\text{splitting in two parts}} + \underbrace{2 \cdot T\left(\frac{n}{2}\right)}_{\text{recursive sort}} \\
&\leq \quad A \cdot n + 2\left(A \cdot \frac{n}{2} + 2 \cdot T\left(\frac{n}{4}\right)\right) \\
&= \quad 2\,A \cdot n + 4 \cdot T\left(\frac{n}{4}\right) \\
&\leq \quad 3\,A \cdot n + 8 \cdot T\left(\frac{n}{8}\right) \\
&\leq \quad \cdots \\
&\leq \quad k \cdot A \cdot n + 2^k \cdot T(1) \\
&= \quad \log_2 n \cdot A \cdot n + n \cdot T(1) \\
&\leq \quad \log_2 n \cdot A \cdot n + n \cdot A \in \mathcal{O}(n \log_2 n)
\end{aligned}
$$

Cache Efficiency

Block Operations - QuickSort

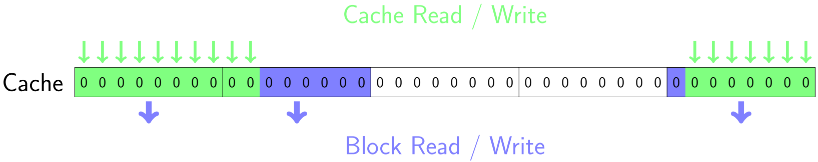


Figure: Locality of quicksort

- Let $IO(n)$ be the number of block operations for input size n
- Assumptions as before but recursion depth is $k = \log_2 \frac{n}{B}$
  Why?

Cache Efficiency

Block Operations - QuickSort

$$
\begin{aligned}
IO(n) \quad &\leq \quad \underbrace{A \cdot n/B}_{\text{splitting in two parts}} \quad + \underbrace{2 \cdot IO\,(n/2)}_{\text{recursive sort}} \\
&\leq \quad A \cdot n/B \quad + \quad 2\,(A \cdot n/2B + 2 \cdot IO\,(n/4)) \\
&\leq \quad 2 \cdot A \cdot n/B \quad + \quad 4 \cdot IO\,(n/4) \\
&\leq \quad 3 \cdot A \cdot n/B \quad + \quad 8 \cdot IO\,(n/8) \\
&\leq \quad \cdots \\
&\leq \quad k \cdot A \cdot n/B \quad + \quad 2^k \cdot IO(n/2^k) \\
&= \quad \log_2(n/B) \cdot A \cdot (n/B) \quad + \quad n/B \cdot IO(B) \\
&\leq \quad \log_2(n/B) \cdot A \cdot (n/B) \quad + \quad A \cdot n/B \quad \in \quad O(\frac{n}{B} \cdot \log_2(\frac{n}{B}
\end{aligned}
$$

Divide and Conquer

Introduction

Concept:

- Divide the problem into smaller subproblems
- Conquer the subproblems through recursive solving.
  If subproblems are small enough solve them directly
- Connect all solutions of the subproblems to a solution of the full problem
- Recursive application of the algorithm to ever smaller subproblems
- Direct solving of sufficently small subproblems

Divide and Conquer

Introduction - Python

- Function solve for solving a problem of size *n*

```python
def solve(problem):
    if n < threshold:
        # solve directly
        return solution
    else:
        # divide problem into subproblems
        # P1, P2, ..., Pk with k>=2
        S1 = solve(P1)
        S2 = solve(P2)
        ...
        Sk = solve(Pk)

        # combine solutions
        return S1 + S2 + ... + Sk
```

Divide and Conquer

Features

- Can help with conceptual hard problems
  - Solution of the trivial problems has to be known
  - Dividing in subproblems has to be possible
  - Combination of solutions has to be possible
- Realization of efficient solutions
  - If trivial solution is $\in O(1)$
  - And separation / combination of subproblems is $\in O(n)$
  - And the number of subproblems is limited
  - The runtime is $\in O(n \cdot \log n)$
- Suitable for parallel processing
  - Subproblems are independent of each other
  - Only needed input for each subproblem has to be known

Divide and Conquer

Implementation

Definition of the trivial case:

- Smaller subproblems are elegant and simple
- Otherwise the efficiency will be improved if relative big subproblems can be solved directly
- Recursion depth should not get too big (stack / memory overhead)

Divide and Conquer

Implementation

Division in subproblems:

- Choosing the number of subproblems and the concrete allocation can be demanding

Combination of solutions:

- Typically conceptional demanding

Divide and Conquer

Example - Maximum Subtotal

Example - Maximum Subtotal Input:

- Progression X of n integers

Output:

- Maximum sum of related subsequence and its index boundary

Index	0	1	2	3	4	5	6	7	8	9
Value	31	-41	59	26	-53	58	97	-93	-23	84

Output: Sum: 187, Start: 2, End: 6

Divide and Conquer

Example - Maximum Subtotal

Application:

- Maximum profit of buying and selling shares

Naive solution (brute force)

```python
def maxSubArray(X):
    # Store sum, start, end
    result = (X[0], 0, 0)
    for i in range(0, len(X)):
        for j in range(i, len(X)):
            subSum = 0
            for k in range(i, j + 1):
                subSum += X[k]
            if result[0] < subSum:
                result = (subSum, i, j)
    return result
```

Runtime - Upper bound

```python
def maxSubArray(X):
    result = (X[0], 0, 0)
    # n loops -> O(n)
    for i in range(0, len(X)):
        # max n loops -> O(n)
        for j in range(i, len(X)):
            # max n loops -> O(n)
            subSum = sum(X[i:j+1])
            if result[0] < subSum: # O(1)
                result = (subSum, i, j)
    return result
```

Upper bound:

- Three interleaved loops
- Each loop with runtime $O(n)$
- Algorithm runtime of $O(n^3)$

Divide and Conquer

Example - Maximum Subtotal - Runtime

Lower bound:

Table: Operations

i	Additions	j
$\frac{n}{3} \in O(n)$	$\frac{n}{3} \in O(n)$	$\frac{n}{3} \in O(n)$

- We iterate at least $\frac{n}{3}$ values for i
- For each i we iterate at least $\frac{n}{3}$ values for j
- For each j we have at least $\frac{n}{3}$ additions
- We need at least $T(n) = (\frac{n}{3})^3 \in \Omega(n^3)$ steps

Runtime:

- With $T(n) \in O(n^3)$ and $T(n) \in \Omega(n^3)$ we know:

$$T(n) \in \Theta(n^3)$$

- It is hard to solve the problem in a worse way ...

Current approach:

- Calculating the sum for range from i to j with loop

$$S_{i,j} = X[i] + X[i+1] + \cdots + X[j]$$

Better approach:

- Incremental sum instead of loop

$$\begin{aligned} S_{i,j+1} &= X[i] + X[i+1] + \cdots + X[j] + X[j+1] \\ S_{i,j+1} &= S_{i,j} + X[j+1] \in O(1) \quad \text{instead of} \quad \in O(n) \end{aligned}$$

Divide and Conquer

Example - Maximum Subtotal - Python

Better solution:

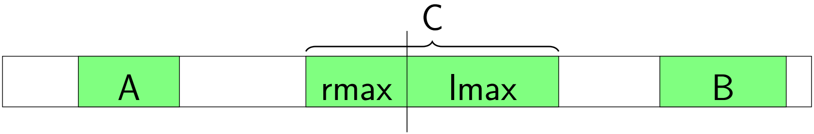
```
def maxSubArray(X):
    result = (X[0], 0, 0)
    # n loops -> O(n)
    for i in range(0, len(X)):
        subSum = 0
        # max n loops -> O(n)
        for j in range(i, len(X)):
            subSum += X[j] # O(1)
            if result[0] < subSum: # O(1)
                result = (subSum, i, j)
    return result
```

- Runtime $\in O(n^2)$

Divide and Conquer

Example - Maximum Subtotal

Divide and Conquer:



Divide and Conquer Idea to solve:

- split the sequence in the middle
- Solve the left half of the problem
- Solve right half and combine both solutions into a total solution
- OK if maximum is located in left half (A) or right half (B)
- Problem: Maximum can overlap split
- To solve this case we have to calculate *rmax* and *lmax*
- The overall solution is the maximum of A, B and C

Divide and Conquer

Example - Maximum Subtotal

Principle - Divide and Conquer:

- Small problems are solved directly: $n = 1 \Rightarrow \max = X[0]$
- Bigger problems are partitioned into two subproblems and recursivly solved. Subsolutions A and B are returned.
- To determine subsolution C, rmax and lmax for the subproblems are computed.
- The overall solution is the maximum of A, B and C

Divide and Conquer

Example - Maximum Subtotal - Python

Divide and conquer solution

```
def maxSubArray(X, i, j):
    if i == j: #trivial case
        return (X[i], i, i)
    m = (i + j) / 2
        #recursive Subsolutions for A,B
    A = maxSubArray(X, i, m)
    B = maxSubArray(X, m + 1, j)
    #rmax and lmax for bordercase C
    C1 = rmax(X, i, m)
    C2 = lmax(X, m + 1, j)
    C = (C1[0] + C2[0], C1[1], C2[1])
    #Solution results from A,B,C
    return max([A, B, C], \
        key=lambda item: item[0])
```

Further Literature

- **General**

[CRL01] Thomas H. Cormen, Ronald L. Rivest, and Charles E. Leiserson.
Introduction to Algorithms.
MIT Press, Cambridge, Mass, 2001.

[MS08] Kurt Mehlhorn and Peter Sanders.
Algorithms and data structures, 2008.
https://people.mpi-inf.mpg.de/~mehlhorn/ftp/Mehlhorn-Sanders-Toolbox.pdf.

Further Literature

- **Caching**

[Wik] Cache
https://en.wikipedia.org/wiki/Cache