Algorithms and Data Structures Runtime analysis Minsort / Heapsort, Induction

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Bioinformatics Group / Department of Computer Science Algorithms and Data Structures, October 2018

Structure



Algorithms and Data Structures

Structure

Links

Organisation

Daphne

Forum

Checkstyle

Unit Tests

Version management

Jenkins

Sorting

Minsort

Heapsort

Topics of the Lecture:

- Algorithms and Data Structures
 Efficient data handling and processing
 ... for problems that occur in practical any larger program / project

Example 1: Sorting



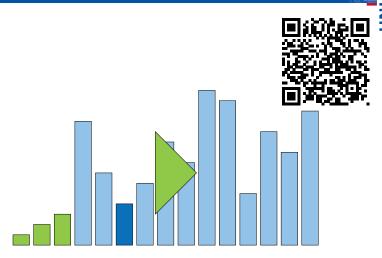


Figure: Sorting with Minsort

- Data structures: How to represent the map as data?
- **Algorithms:** How to find the shortest / fastest way?

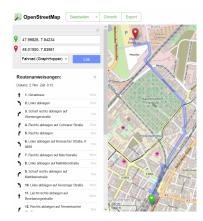


Figure: Navigationplan © OpenStreetMap

Example 3: Fault Tolerant Search







Ergebnisse für eyjafjallajökull

Stattdessen suchen nach: ejafjatlajökuk

Eyjafjallajökull - Wikipedia

de.wikipedia.org/wiki/Eyjafjallajökull 🔻

Der Name Eyjafjallajökull (islandisch für "Inselberge-Gletscher") rührt von den so genannten Landeyjar (dt. Landinseln) her. Das sind felsige Erhebungen, ... Name - Der Gletscher - Der Vulkan unter dem Gletscher - Eruptionsgeschichte

Eyjafjallajökull - Der unaussprechliche Vulkanfilm Film 2014 ...

31.07.2014 - **Eyjafjallajökull** - Der unaussprechliche Vulkanfilm, Irwitzige Komödie um ein verfeindetes Ex-Eheoaar, das wegen der Asche des isländischen ...

Bilder zu eyjafjallajökull

Unangemessene Bilder melden











Eyjafjallajökull

Gletscher in Island

Der Eyjafjallajókull, zu deutsch Eyjafjöll-Gletscher, ist der sechstgrößte Gletscher Islands. Er liegt an der außersten Südküste, westlich des Gletschers Myrdalsjökull in der Gemeinde Rangárþing eystra, die größte Höhe beträgt 1651 m. Wikipedia

Letzte Eruption: April 2010 Höhe: 1 666 m

Fläche: 100 km²

Prominenz: 1.051 m

■ Edit Distance: game changer in molecular biology

Gapped BLAST and PSI-BLAST: a new generation of protein database search programs SF Altschul, TL Madden, AA Schäffer... - Nucleic acids ..., 1997 - Oxford Univ Press

Abstract The **BLAST** programs are widely used tools for searching protein and DNA databases for sequence similarities. For protein comparisons, a variety of definitional, algorithmic and statistical refinements described here permits the execution time of the ... Zitiert von: 55822 Ahnliche Artikel Alle 148 Versionen Zitieren Speichern

► NCBI/ BLAST/ blastp st	uite	Standard Protein BLAST				
blastn blastp blastx	tblastn tblastx					
Enter Query Se	equence BLA	LASTP programs search protein databases using a protein query. more				
Enter accession nu	umber(s), gi(s), or FASTA sequence(s) 🤢	Clear Query subrange 😡				
[Arabidopsis tha	VLFAAFDAPAMVEAQKLCEKPSGTWSGVCGNSNACKNQCINLEGAKHGS	From				
Or, upload file	Bestand kiezen Geen bestand gekozen 🧼					
000 1100	gi[15241496]ref[NP_199255.1] defensin-like Enter a descriptive title for your BLAST search					
Align two or mo	ore sequences 😥					
Choose Search	th Set					
Database		• •				
	Title: Non-redundant UniProtKB/SwissProt sequence Molecule Type: Protein	inces.				



General:

- Most of you had a lecture on basic programming ... performance was not an issue
- Here it is going to be:
 - How fast is our program?
 - 2 How can we make it faster?
 - 3 How can we proof that it will always be that fast?
- Important issues:
 - Most of the time: application runtime
 - Sometimes also: resource / space consumption

Algorithms:

- Sorting
- Dynamic Arrays
- Associative Arrays
- Hashing
- Edit distance

- Priority Queue
- Linked Lists
- Pathfinding / Dijkstra Algorithm
- Search Trees

Mathematics:

- Runtime analysis
- Ø-Notation

Proof of correctness

■ ... you should be able to understand the joke

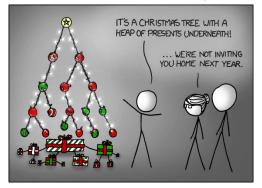


Figure: Comic @ xkcd/835

Hopefully your parents will still invite you



Homepage:

- Exercise sheets
- Lectures
- Materials

Link to Homepage

Lecture:

- Tuesday, 12:00 14:00, HS 00 006, Build. 082
- Recordings of the lecture will be uploaded to the webpage

Exercises:

- One exercise sheet per week
- Submission / Correction / Assistance online
- Tutorial: (if needed)Wednesday, 13:00-14:00 HS 00 006, Build. 082

Exam:

■ Planned: Sa. 23th March 2019, 10:00-12:00, Build. 101, Lec. theater 026 & 036

Exercises:

- 80% practical, 20% theoretical
- We expect **everyone** to solve **every** exercise sheet

Exam:

- 50% of all points from the exercise sheets are needed
- Content of exam: whole lecture and all exercises

Exercises:

- Tutors: Tim Maffenbeier, Till Steinmann, Tobias Faller
- Coordinators: Michael Uhl, Florian Eggenhofer and Björn Grüning
- Deadline: ESE: 1 week, IEMS: none

Exercises:

- Post questions into the forum (link later)
- Submission via "commit" through svn and Daphne
- Feedback one week after deadline through "update" (svn)
- Unit test / checkstyle via Jenkins

Exercises - Points:

- Practical:
 - 60% functionality
 - 20% tests
 - 20% documentation, Checkstyle, etc.
 - Program is not running ⇒ 0 points
- Theoretical (mathematical proof):
 - 40% general idea / approach
 - 60% clean / complete

Effort:

- 4 ECTS (ESE), 6 ECTS (IEMS)
- 120 / 180 working hours per semester
- 14 Lectures each 6h / 8h + exam
- 4h / 6h per exercise sheet (one per week)

Daphne:

- Provides the following information:
 - Name / contact information of your tutor
 - Download of / info needed for exercise sheets
 - Collected points of all exercise sheets
 - Links to:
 - Coding standards
 - 2 Build system
 - 3 The other systems
- Link: Daphne

Forum:

- Please don't hesitate to ask if something is unclear
- Ask in the forum and not separate. Others might also be interested in the answer
- The tutors or the coordinators will reply as soon as possible
- Link: Forum

Checkstyle / Linting (flake8):

■ Installation: python3 -m pip install flake8

■ Check file: python3 -m flake8 path/to/files/*.py

■ Link: flake8

Why unit tests?

- A non-trivial method without a unit test is probably wrong
- Simplifies debugging
- We and you can automatically check correctness of code

What is a good unit test?

- Unit test checks desired output for a given input
- At least one typical input
- At least one critical case
 E.g. double occurrence of a value in sorting

Testing (doctest):

```
def subtract one(n):
    """Subtracts 1 from n
    >>> subtract one(5)
    >>> subtract one(3)
    ....
    return n-1
if __name__ == "__main__":
```

- Tests are contained in docstrings
- Module doctest runs them
- Run check with: python3 -m doctest path/to/files/*.py -v

```
f __name__ == "__main__":
    print("2 - 1 = %d" % subtract_one(2))
```

Version management (subversion):

- Keeps a history of code changes
- Initialize / update directory: **svn** checkout <URL>
- Add files / folders: svn add <file> --all
- Create snapshot: **svn** commit -m "<Your Message>" Data is uploaded to Jenkins automatically
- Link: Subversion

Jenkins:

- Provides our build system
- You can check if your uploded code runs
 - Especially whether all unit test pass
 - And if checkstyle (flake8) is statisfied
- Will be shown in the first exercise
- Link: Jenkins

Problem:

- Input: n elements $x_1, ..., x_n$
- Transitive operator "<" which returns true if the left value is smaller than the right one
 - Transitivity: x < y, $y < z \rightarrow x < z$
- Output: x_1, \dots, x_n sorted with operator

Example

Input: 14, 4, 32, 19, 8, 44, 65

Output:

Why do we need sorting?

- Nearly every program needs a sorting algorithm
- **Examples:**
 - Index of a search engine
 - Listing filesystem in explorer / finder
 - (Music) library
 - Highscore list

Informal description:

- Find the minimum and switch the value with the first position
- Find the minimum and switch the value with the second position

...

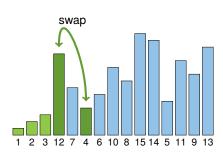


Figure: Minsort

Minsort in Python:

```
def minsort(lst):
    for i in range(0, len(lst)-1):
        minimum = i
        for j in range(i+1, len(lst)):
             if lst[j] < lst[minimum]:</pre>
                 minimum = i
        if minimum != i:
             [st[i], [st[minimum] = \]
                 Ist[minimum], Ist[i]
    return 1st
```



How long does our program run?

- We test it for different input sizes
- Observation: It is going to be "disproportionately" slower the more numbers are being sorted

Table: Runtime for Minsort

n	Runtime / ms		
2 × 10 ³	5.24		
4×10^3	16.92		
6×10^3	39.11		
8×10^3	67.80		
10×10^3	105.50		
12×10^3	150.38		
14×10^3	204.00		
16×10^3	265.98		
18×10^3	334.94		

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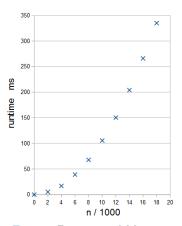


Figure: Runtime of *Minsort*

Runtime analysis:

- Minsort runtime depicted in a diagram
 - That is what you should do in the first exercise sheet

We observe:

- The runtime grows faster than linear
- With double the input size we need four times the time

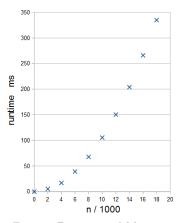


Figure: Runtime of *Minsort*

Heapsort:

- The principle stays the same
- Better structure for finding the smallest element quicker

Binary heap:

- Preferably a complete binary tree
- **Heap property:** Each child is smaller (larger) than the parent element

Min heap:

- **Heap property:** Each child is smaller (larger) than the parent element
- A valid heap fulfills the property at each node

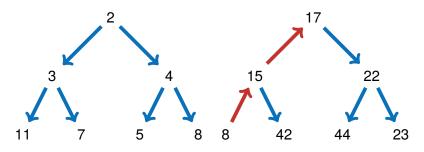
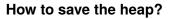


Figure: Valid min heap

Figure: Invalid min heap



- We number all nodes from top to bottom and left to right starting at 0
 - The children of node i are 2i + 1 and 2i + 2
 - The parent node of node *i* is floor $\left(\frac{i-1}{2}\right)$

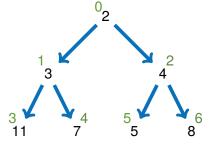


Table: Elements can be stored in array

0	1	2	3	4	5	6
2	3	4	11	7	5	8

Heapsort - Algorithm 4 / 10

Repairing after taking the smallest element: heap.pop()

- Remove the smallest element (root node)
- Replace the root with the last node
- Sift the new root node down until the heap property is satisfied

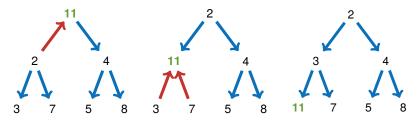


Figure: Repairing a min heap via sifting



Heapsort:

- Organize the *n* elements as heap
- While the heap still contains elements
 - Take the smallest element
 - Move the last node to the root
 - Repair the heap as described
- Output: 2, 3, ...

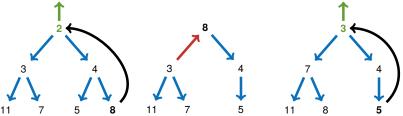
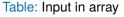


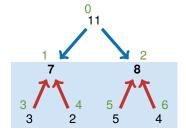
Figure: One iteration of Heapsort

Creating a heap:

- This operation is called heapify
- The n elements are already stored in an array
- Interpret the array as binary heap where the heap property is not yet satisfied
- We repair the heap from bottom up (in layers) with sifting



0	1	2	3	4	5	6
11	7	8	3	2	5	4



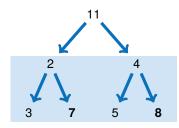
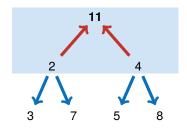


Figure: Heapify lower layer



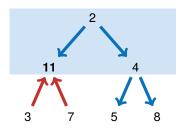


Figure: Heapify upper layer

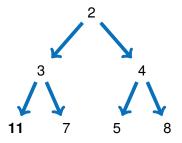


Figure: Resulting heap

Finding the minimum is intuitive:

- Minsort: Iterate through all non-sorted elements
- **Heapsort:** Finding the minimum is trivial (concept)

 Just take the root of the heap

Removing the minimum in Heapsort:

- Repair the heap and restore the heap property
 - We don't have to repair the whole heap
- More of this in the next lecture

■ Course literature

[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.
Springer, Berlin, 2008.
https://people.mpi-inf.mpg.de/~mehlhorn/
ftp/Mehlhorn-Sanders-Toolbox.pdf.

Sorting

[Wika] Wikipedia - Heapsort

https://en.wikipedia.org/wiki/Heapsort

[Wikb] Wikipedia - Selectionsort

https://de.wikipedia.org/wiki/Selectionsort

Further Literature



Subversion

[Apa] Apache Subversion

https://subversion.apache.org/