Algorithms and Data Structures Runtime analysis Minsort / Heapsort, Induction

Prof. Dr. Rolf Backofen

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

Algorithms and Data Structures

Topics of this Lecture

Topics of the Lecture:

- Algorithms and Data Structures
 Efficient data handling and processing
 ... for problems that occur in practical any larger program / project
- ► **Algorithm** Solving of complex computional problems

Example 1: Sorting

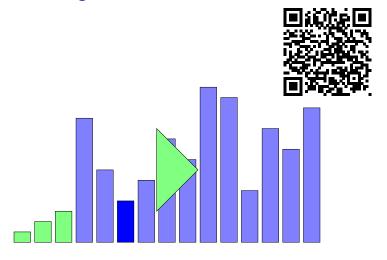


Figure: Sorting with Minsort

Example 2: Navigation

- ▶ 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



Eyjafjallajökull - Der unaussprechliche Vulkanfilm Film 2014 ... www.kino.de > Filme >

31.07.2014 - Eyjafjallajökull - Der unaussprechliche Vulkanfilm, Irrwitzige Komödie um ein verfeindetes Ex-Ehepaar, das wegen der Asche des isländischen ...

Bilder zu eviafiallajökull

Unangemessene Bilder melden









Weitere Bilder zu eviafiallaiökull

Eyjafjallajökull

Gletscher in Island

Der Evjafjallajökull, zu deutsch Evjafjöll-Gletscher, ist der sechstgrößte Gletscher Islands. Er liegt an der äußersten Südküste westlich des Gletschers Mýrdalsjökull 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

Erstbesteiger: Sveinn Pálsson

Example 4: Protein Search

Edit Distance: game changer in molecular biology

Gapped BLAST and PSI-BLAST: a new generation of protein database search programs

<u>SF Altschul</u>, <u>TL Madden</u>, <u>AA Schäffer</u>... - 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 Ähnliche Artikel Alle 148 Versionen Zitieren Soeichern

► NCBI/ BLAST/ blastp suite		Standard Protein BLAST				
blastn blastp blasts	tblastn tblastx					
Enter Query Se	equence BLA	ASTP programs search protein databases using a protein query. more				
Enter accession n	umber(s), gi(s), or FASTA sequence(s) 🤢	Clear Query subrange 🤢				
[Arabidopsis the	LFAAFDAPAMVEAQKLCEKPSGTWSGVCGNSNACKNQCINLEGAKHGS	From				
Or, upload file Job Title	Bestand kiezen Geen bestand gekozen gil 15241496 jrefi NP_199255. 1 j defensin-like Enter a derpitive title for your BLAST search green progress.					
Choose Searc						
Database						
	Title: Non-redundant UniProtKB/SwissProt sequenc Molecule Type: Protein Update date: 2013/03/23 Number of sequences: 454721	ces.				
Organism Optional	Enter organism common name, binomial, or tax id. Only 20	☐ Exclude				

Content of the Lecture 1 / 2

General:

- ► Most of you had a lecture on basic progamming . . . performance was not an issue
- Here it is going to be:
 - 1. 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

Content of the Lecture 2 / 2

Algorithms:

- Sorting
- Dynamic Arrays
- Associative Arrays
- Hashing
- ► Edit distance
- Mathematics:
- Runtime analysis
- ► O-Notation

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

Proof of correctness

After the lecture . . .

... you should be able to understand the joke

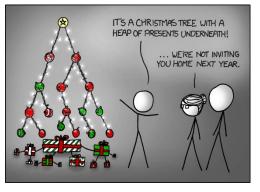


Figure: Comic © xkcd/835

► Hopefully your parents will still invite you

Links



Homepage:

- Exercise sheets
- Lectures
- Materials

Link to Homepage

Organisation 1 / 5

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

Organisation 2 / 5

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

Organisation - Exercises 3 / 5

Exercises:

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

Organisation - Exercises 3 / 5

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

Organisation - Exercises 4 / 5

Exercises - Points:

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

Organisation 5 / 5

Effort:

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

Daphne

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:
 - 1. Coding standards
 - 2. Build system
 - 3. The other systems
- ► Link: Daphne

Forum

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 flake8

Checkstyle / Linting (flake8):

▶ Installation: python3 -m pip install flake8

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

► Link: flake8

Unit Tests

Why unit tests?

- 1. A non-trivial method without a unit test is probably wrong
- 2. Simplifies debugging
- 3. 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

Unit Tests

doctest

Testing (doctest):

def subtract_one(n):

```
""" Subtracts 1 from n

>>> subtract_one(5)
4

>>> subtract_one(3)
2
"""
return n-1
```

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

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

Version management

Subversion

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

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

Sorting 1 / 2

Problem:

- ▶ Input: n elements x_1, \ldots, 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: $x_1, ..., x_n$ sorted with operator

Example

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

Output:

Sorting 2 / 2

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

Minsort - Algorithm

Informal description:

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

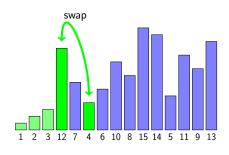


Figure: Minsort

Minsort - Algorithm

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 = j
         if minimum != i:
             lst[i], lst[minimum] = \
                 Ist [minimum], Ist [i]
    return Ist
```

Minsort - Runtime

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
$14 imes 10^3$	204.00
$16 imes 10^3$	265.98
18×10^3	334.94

Minsort - Runtime

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

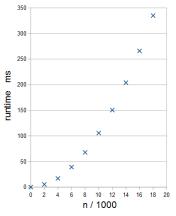


Figure: Runtime of Minsort

Minsort - Runtime

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

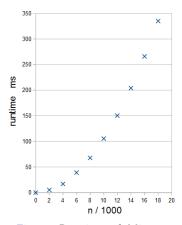


Figure: Runtime of Minsort

► Next lecture we will analyze deeper with other methods

Heapsort - Algorithm 1 / 10

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

Heapsort - Algorithm 2 / 10

Min heap:

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

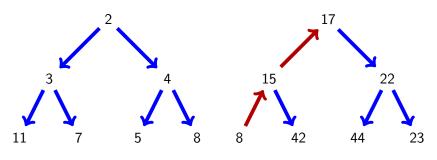


Figure: Valid min heap

Figure: Invalid min heap

Heapsort - Algorithm 3 / 10

How to save the 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 $\left(\frac{i-1}{2}\right)$

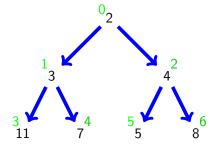


Table: Elements can be stored in array

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

Figure: Min heap

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

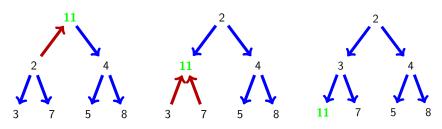


Figure: Repairing a min heap via sifting

Heapsort - Algorithm 5 / 10

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, ...

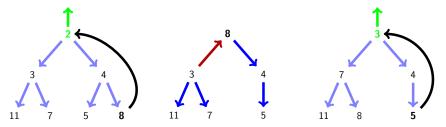


Figure: One iteration of Heapsort

Heapsort - Algorithm 6 / 10

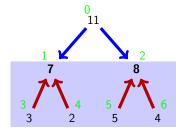
Creating a heap:

- ► This operation is called heapify
- ightharpoonup 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

Heapsort - Algorithm 7 / 10

Table: Input in array

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



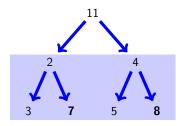
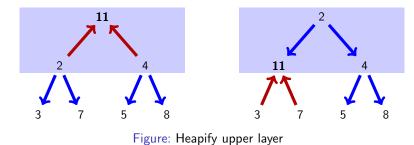


Figure: Heapify lower layer

Heapsort - Algorithm 8 / 10



Heapsort - Algorithm 9 / 10

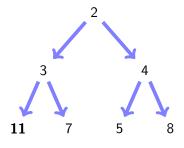


Figure: Resulting heap

Heapsort - Algorithm 10 / 10

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

Further Literature

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.

Further Literature

Sorting

Further Literature

Subversion

```
[Apa] Apache Subversion
https://subversion.apache.org/
```