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

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Algorithms and Data Structures

Topics of this Lecture

Topics of the Lecture:

► Algorithms and Data Structures

- ightharpoonup Algorithm $\hat{=}$ Solving of complex computional problems

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
- **▶ Data structure** *â* Representation of data on computer

Example 1: Sorting

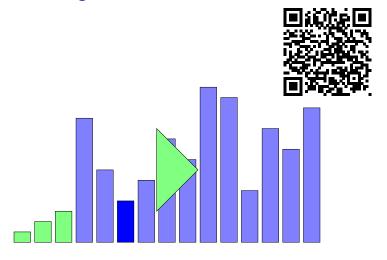


Figure: Sorting with Minsort

Example 2: Navigation



Figure: Navigationplan © OpenStreetMap

Example 2: Navigation

▶ Data structures: How to represent the map as data?

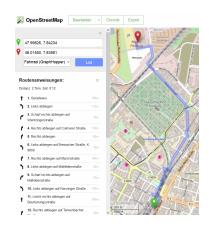


Figure: Navigationplan © OpenStreetMap

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.s.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 s	uite	Standard Protein BLAST
blastn blastp blasts	tblastn tblastx	
Enter Query Se	equence	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 gregoringers.	
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 to	Exclude •

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General:

► Most of you had a lecture on basic progamming . . . performance was not an issue

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- 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

Algorithms:

Algorithms:

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

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

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Mathematics:

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

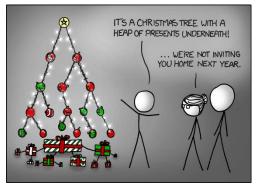


Figure: Comic © xkcd/835

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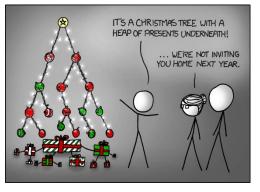


Figure: Comic © xkcd/835

► Hopefully your parents will still invite you

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Homepage:

- Exercise sheets
- Lectures
- Materials

Link to Homepage

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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

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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

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- ▶ Deadline: ESE: 1 week, IEMS: none

Exercises:

▶ Post questions into the forum (link later)

Organisation - Exercises 3 / 5

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Organisation - Exercises 3 / 5

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- ► Feedback one week after deadline through "update" (svn)

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

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)

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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

Why unit tests?

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Unit test checks desired output for a given input

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- At least one typical input

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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

doctest

Testing (doctest):

```
Tests are contained in
def subtract_one(n):
    """ Subtracts 1 from n
                                   docstrings
   >>> subtract_one(5)
    4
   >>> subtract_one(3)
    return n-1
if __name__ == "__main__":
    print("2 - 1 = \%d" \% subtract_one(2))
```

doctest

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doctest

Testing (doctest):

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```
""" 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

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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

Sorting 1 / 2

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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

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Informal description:

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

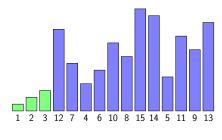


Figure: Minsort

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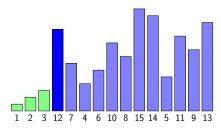


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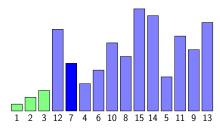
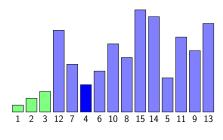


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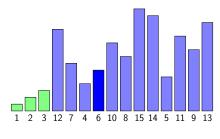
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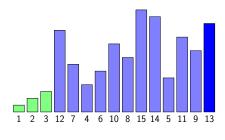
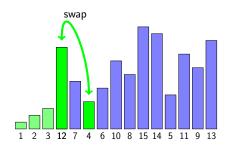


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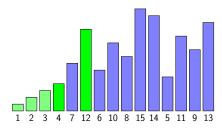
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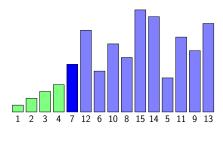
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Minsort - Algorithm

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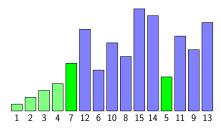


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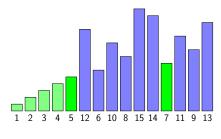


Figure: Minsort

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
```

How long does our program run?

We test it for different input sizes

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Tah	ا حوا	Puntime	for	Minsort
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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
16×10^3	265.98
18×10^3	334.94

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
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Table: Runtime for Minsort

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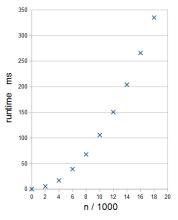


Figure: Runtime of Minsort

Runtime analysis:

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

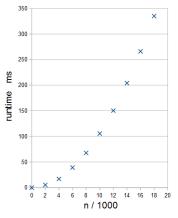


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Runtime analysis:

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 - With double the input size we need four times the time

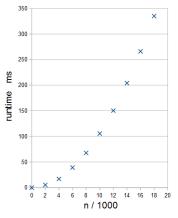


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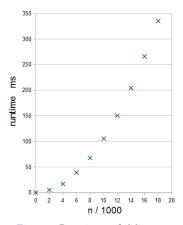


Figure: Runtime of Minsort

► Next lecture we will analyze deeper with other methods

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

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

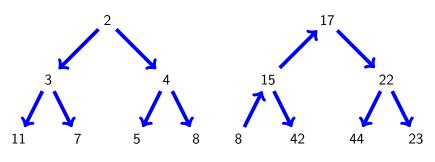


Figure: Valid min heap Figure: Invalid min heap

Min heap:

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

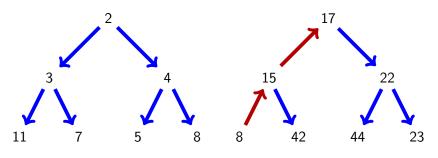


Figure: Valid min heap

Figure: Invalid min heap

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 $\left(\frac{i-1}{2}\right)$

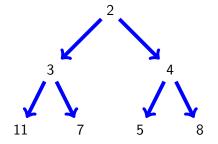


Table: Elements can be stored in array

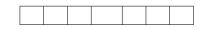


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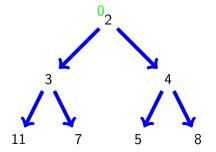


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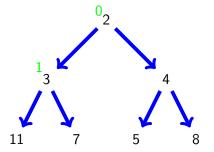


Table: Elements can be stored in array

0	1			
2	3			

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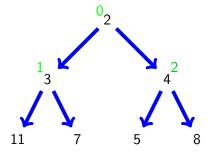


Table: Elements can be stored in array

0	1	2		
2	3	4		

Figure: Min heap

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 $\left(\frac{i-1}{2}\right)$

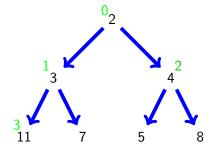


Table: Elements can be stored in array

0	1	2	3		
2	3	4	11		

Figure: Min heap

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 $\left(\frac{i-1}{2}\right)$

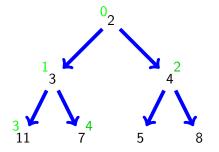


Table: Elements can be stored in array

0	1	2	3	4	
2	3	4	11	7	

Figure: Min heap

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 $\left(\frac{i-1}{2}\right)$

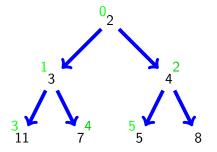


Table: Elements can be stored in array

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

Figure: Min heap

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 $\left(\frac{i-1}{2}\right)$

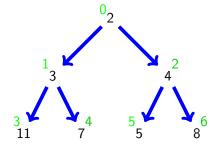


Table: Elements can be stored in array

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

Figure: Min heap

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

► Remove the smallest element (root node)

- Remove the smallest element (root node)
- Replace the root with the last node

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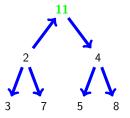


Figure: Repairing a min heap via sifting

- Remove the smallest element (root node)
- Replace the root with the last node
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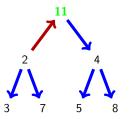


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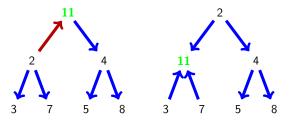


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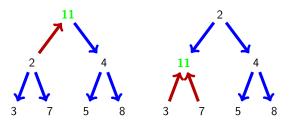


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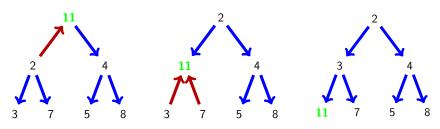


Figure: Repairing a min heap via sifting

- 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

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- While the heap still contains elements
 - ► Take the smallest element
 - ► Move the last node to the root
 - Repair the heap as described
- ► Output: 2

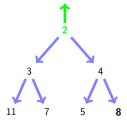


Figure: One iteration of Heapsort

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- ► Output: 2

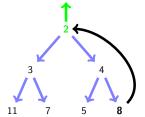


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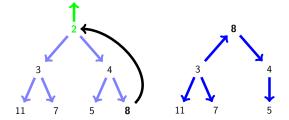


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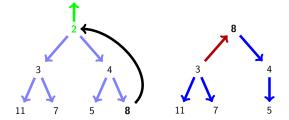


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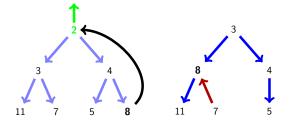


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- Output: 2

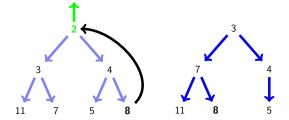


Figure: One iteration of Heapsort

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- While the heap still contains elements
 - Take the smallest element
 - ► Move the last node to the root
 - Repair the heap as described
- ► Output: 2

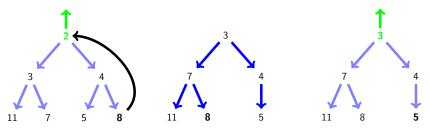


Figure: One iteration of Heapsort

- 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, ...

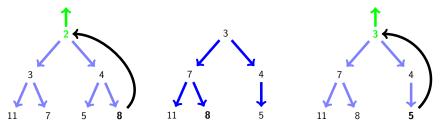


Figure: One iteration of Heapsort

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- 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

Table: Input in array

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

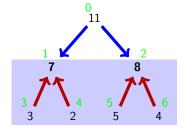
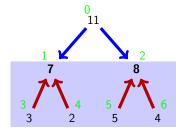


Figure: Heapify lower layer

Table: Input in array

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



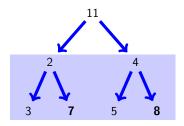


Figure: Heapify lower layer

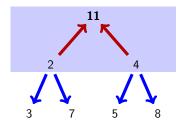
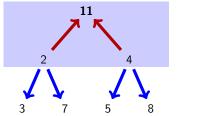


Figure: Heapify upper layer



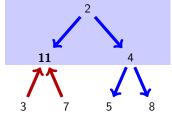


Figure: Heapify upper layer

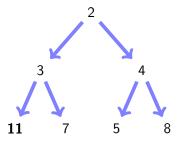


Figure: Resulting heap

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

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- 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/
```