Advanced Algorithms and Data Structures (WS 2023/24)

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October 12, 2023

UNIVERSITÄT SALZBURG
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Personalia

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Formalia

URL of course (VO+PS):	Base-URL`/teaching/aads/aads.html`.
Lecture times (VO):	Thursday 8^{00}–11^{10} (with a break of about 20 minutes).
Venue (VO):	PLUS, Informatik, T03, Jakob-Haringer Str. 2.
Lecture times (PS):	Thursday 12^{00}–14^{00}.
Venue (PS):	PLUS, Informatik, T03, Jakob-Haringer Str. 2.

Note — PS is graded according to continuous-assessment mode!

Electronic Slides and Online Material

In addition to these slides, you are encouraged to consult the WWW home-page of this lecture:

https://www.cosy.sbg.ac.at/˜held/teaching/aads/aads.html.

In particular, this WWW page contains up-to-date information on the course, plus links to online notes, slides and (possibly) sample code.

A Few Words of Warning

- I hope that these slides will serve as a practice-minded introduction to various aspects of advanced algorithms and data structures. I would like to warn you explicitly not to regard these slides as the sole source of information on the topics of my course. It may and will happen that I'll use the lecture for talking about subtle details that need not be covered in these slides! In particular, the slides won't contain all sample calculations, proofs of theorems, demonstrations of algorithms, or solutions to problems posed during my lecture. That is, by making these slides available to you I do not intend to encourage you to attend the lecture on an irregular basis.
- See also In Praise of Lectures by T.W. Körner.
- A *basic knowledge of algorithms, data structures, elementary probability theory, and discrete mathematics*, as taught typically in undergraduate courses, should suffice to take this course. It is my sincere intention to start at a suitable hypothetical level of "typical prior undergrad knowledge". Still, it is obvious that different educational backgrounds will result in different levels of prior knowledge. Hence, you might realize that you do already know some items covered in this course, while you lack a decent understanding of some items which I seem to presuppose. In such a case I do expect you to refresh or fill in those missing items on your own!

Acknowledgments

A small portion of these slides is based on notes and slides produced by students and colleagues — most notably Therese Biedl, Jeff Erickson, Pat Morin's "Open Data Structures", Paolo di Stolfo, Peter Palfrader — on topics related to algorithms and data structures. I would like to express my thankfulness to all of them for their help. This revision and extension was carried out by myself, and I am responsible for all errors.

I am also happy to acknowledge that I benefited from material published by colleagues on diverse topics that are partially covered in this lecture. While some of the material used for this lecture was originally presented in traditional-style publications (such as textbooks), some other material has its roots in non-standard publication outlets (such as online documentations, electronic course notes, or user manuals).

Salzburg, August 2023 Martin Held

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Recommended Textbooks for Background Reading I

- T.H. Cormen, C.E. Leiserson, R.L. Rivest, C. Stein.
  Introduction to Algorithms.
  MIT Press, 4th edition, April 2022; ISBN 978-0262046305.
- J. Kleinberg, É. Tardos.
  Algorithm Design.
  Pearson, 2013; ISBN 978-1292023946.
- S.S. Skiena.
  The Algorithm Design Manual.
  Springer, 3rd edition, Oct 2020; ISBN 978-3030542559.
  `https://www.algorist.com/`
- D.E. Knuth.
  The Art of Computer Programming. Vol. 1: Fundamental Algorithms.
  Addison-Wesley, 3rd edition, 1997; 978-0201896831.
- D.E. Knuth.
  The Art of Computer Programming. Vol. 3: Sorting and Searching.
  Addison-Wesley, 2nd edition, 1998; 978-0201896855.

Recommended Textbooks for Background Reading II

- J. Erickson.
  Algorithms.
  June 2019; ISBN 978-1792644832.
  `https://jeffe.cs.illinois.edu/teaching/algorithms/`
- P. Brass.
  Advanced Data Structures.
  Cambridge Univ. Press, 2008; ISBN 978-0521880374.
  `https://www-cs.ccny.cuny.edu/~peter/dstest.html`
- P. Morin.
  Open Data Structures.
  `https://opendatastructures.org/`
- D. Sheehy.
  datastructures.
  `https://donsheehy.github.io/datastructures/`
- Community effort.
  OpenDSA.
  `https://opendsa-server.cs.vt.edu/`

Table of Content

Introduction

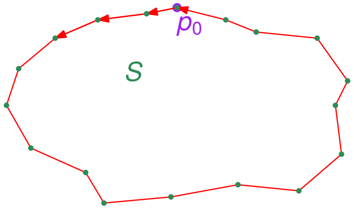
It's Obvious!?

Problem: EUCLIDEANTRAVELINGSALESMANPROBLEM (ETSP)

Input: A set S of n points in the Euclidean plane.

Output: A cycle of minimum length that starts and ends in one point of S and visits all points of S.

- Natural strategy to solve an instance of ETSP:
  1. Pick a point $p_0 \in S$.
  2. Find its nearest neighbor $p' \in S$, move to p', and let $p := p'$.
  3. Continue from p to the nearest unvisited neighbor $p' \in S$ of p, and let $p := p'$.
  4. Repeat the last step until all points have been visited, and return back to p_0.

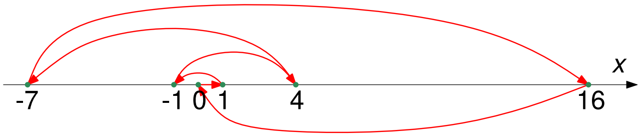


It's Obvious!?

- The strategy to always pick the shortest missing link can be seen as a *greedy* strategy. (More on greedy strategies later during this course.)
- It is obvious that this strategy will always solve ETSP, isn't it?
- Well . . . The tour computed need not even be close in length to the optimum tour!
- In the example, the tour computed has length 58, while the optimum tour has length 46!

Intuition . . .

. . . is important, but it may not replace formal reasoning. Intuition might misguide, and algorithm design without formal reasoning does not make sense.



Will it Terminate?

Caveat

Even seemingly simple algorithms need not be easy to understand and analyze.

```
void Collatz(int n)
{
   while (n>1) {
      if (ODD(n)) n := 3n + 1;
      else        n := n / 2;
   }
   printf("done!\n");
   return;
}
```

- It is not known whether the so-called Collatz $3n + 1$ recursion [Collatz 1937] will terminate for all $n \in \mathbb{N}$.
- Conjecture: It terminates for all $n \in \mathbb{N}$.
- Obviously $T(2^k) = 1$ after k steps for all $k \in \mathbb{N}_0$.
- Experiments have confirmed the Collatz conjecture up to $2^{68} \approx 2.95 \cdot 10^{20} \dots$

Notation

- Numbers:
  - The set $\{1, 2, 3, \ldots\}$ of natural numbers is denoted by $\mathbb{N}$, with $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$.
  - The set $\{2, 3, 5, 7, 11, 13, \ldots\} \subset \mathbb{N}$ of prime numbers is denoted by $\mathbb{P}$.
  - The (positive and negative) integers are denoted by $\mathbb{Z}$.
  - $\mathbb{Z}_n := \{0, 1, 2, \ldots, n-1\}$ and $\mathbb{Z}_n^+ := \{1, 2, \ldots, n-1\}$ for $n \in \mathbb{N}$.
  - The reals are denoted by $\mathbb{R}$; the non-negative reals are denoted by $\mathbb{R}_0^+$, and the positive reals by $\mathbb{R}^+$.
- Open or closed intervals $I \subset \mathbb{R}$ are denoted using square brackets: e.g., $I_1 = [a_1, b_1]$ or $I_2 = [a_2, b_2[$, with $a_1, a_2, b_1, b_2 \in \mathbb{R}$, where the right-hand "[" indicates that the value b_2 is not included in I_2.
- The set of all elements $a \in A$ with property $P(a)$, for some set A and some predicate P, is denoted by

$$\{x \in A : \; P(x)\} \quad \text{or} \quad \{x : x \in A \wedge \; P(x)\}$$

or

$$\{x \in A \mid P(x)\} \quad \text{or} \quad \{x \mid x \in A \wedge \; P(x)\}.$$

- Bold capital letters, such as **M**, are used for matrices.
- The set of all (real) $m \times n$ matrices is denoted by $M_{m \times n}$.

Notation

- Points are denoted by letters written in italics: p, q or, occasionally, P, Q. We do not distinguish between a point and its position vector.
- The coordinates of a vector are denoted by using indices (or numbers): e.g., $v = (v_x, v_y)$ for $v \in \mathbb{R}^2$, or $v = (v_1, v_2, \dots, v_n)$ for $v \in \mathbb{R}^n$.
- In order to state $v \in \mathbb{R}^n$ in vector form we will mix column and row vectors freely unless a specific form is required, such as for matrix multiplication.
- The vector dot product of two vectors $v, w \in \mathbb{R}^n$ is denoted by $\langle v, w \rangle$. That is, $\langle v, w \rangle = \sum_{i=1}^{n} v_i \cdot w_i$ for $v, w \in \mathbb{R}^n$.
- The vector cross-product (in $\mathbb{R}^3$) is denoted by a cross: $v \times w$.
- The length of a vector v is denoted by $\|v\|$.
- The straight-line segment between the points p and q is denoted by $\overline{pq}$.
- The supporting line of the points p and q is denoted by $\ell(p, q)$.
- The cardinality of a set A is denoted by $|A|$.
- Quantifiers: The universal quantifier is denoted by $\forall$, and $\exists$ denotes the existential quantifier.

Terminology

- Unfortunately, the terminology used in textbooks and research papers on algorithms and data structures often lacks a rigorous standardization.
- This comment is particularly true for the underlying graph theory!
- We will rely on the terminology and conventions used in my course on “Discrete Mathematics”.

Advice

Please make sure to familiarize yourself with the terminology and conventions used in “Discrete Mathematics”!

Logarithms

Definition 1 (*Logarithm*)

The *logarithm* of a positive real number $x \in \mathbb{R}^+$ with respect to a base b, which is a positive real number not equal to 1, is the unique solution y of the equation $b^y = x$. It is denoted by $\log_b x$.

- Hence, it is the exponent by which b must be raised to yield x.
- Common bases:

$$\operatorname{ld} x := \log_2 x \qquad \ln x := \log_e x \quad \text{with} \quad e := \lim_{n\to\infty}\left(1+\frac{1}{n}\right)^n \approx 2.71828\ldots$$

Lemma 2

Let $x, y, p \in \mathbb{R}^+$ and $b \in \mathbb{R}^+ \setminus \{1\}$.

$$\log_b(xy) = \log_b(x) + \log_b(y) \qquad \log_b\left(\frac{x}{y}\right) = \log_b(x) - \log_b(y)$$

$$\log_b\left(x^p\right) = p\log_b(x) \qquad \log_b\left(\sqrt[p]{x}\right) = \frac{\log_b(x)}{p}$$

Logarithms

Lemma 3 (*Change of base*)

Let $x \in \mathbb{R}^+$ and $\alpha, \beta \in \mathbb{R}^+ \setminus \{1\}$. Then $\log_\alpha(x)$ and $\log_\beta(x)$ differ only by a multiplicative constant:

$$\log_\alpha(x) = \frac{1}{\log_\beta(\alpha)} \cdot \log_\beta(x)$$

Convention

In this course, $\log n$ will always denote the logarithm of n to the base 2, i.e., $\log n := \log_2 n$.

Fibonacci Numbers

Definition 4 (*Fibonacci numbers*)

For all $n \in \mathbb{N}_0$,

$$F_n := \begin{cases} n & \text{if } n \leq 1, \\ F_{n-1} + F_{n-2} & \text{if } n \geq 2. \end{cases}$$

n	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
F_n	0	1	1	2	3	5	8	13	21	34	55	89	144	233	377	610

Lemma 5

For $n \in \mathbb{N}$ with $n \geq 2$:

$$F_n = \frac{1}{\sqrt{5}} \cdot \left(\frac{1+\sqrt{5}}{2}\right)^n - \frac{1}{\sqrt{5}} \cdot \left(\frac{1-\sqrt{5}}{2}\right)^n \geq \left(\frac{1+\sqrt{5}}{2}\right)^{n-2}$$

- Lots of interesting mathematical properties. For instance,

$$\lim_{n\to\infty} \frac{F_{n+1}}{F_n} = \phi, \quad \text{where } \phi := \frac{1+\sqrt{5}}{2} = 1.618\ldots \text{ is the } \textit{golden ratio}.$$

Catalan Numbers

Definition 6 (*Catalan numbers*)

For $n \in \mathbb{N}_0$,

$$C_0 := 1 \quad \text{and} \quad C_{n+1} := \sum_{i=0}^{n} C_i \cdot C_{n-i}.$$

n	0	1	2	3	4	5	6	7	8	9	10	11
C_n	1	1	2	5	14	42	132	429	1430	4862	16796	58786

Lemma 7

For $n \in \mathbb{N}_0$,

$$C_n = \frac{1}{n+1} \sum_{i=0}^{n} \binom{n}{i}^2 = \frac{1}{n+1} \binom{2n}{n} \in \Theta\left(\frac{4^n}{n^{1.5}}\right).$$

Harmonic Numbers

Definition 8 (*Harmonic numbers*)

For $n \in \mathbb{N}$,

$$H_n := 1 + \frac{1}{2} + \frac{1}{3} + \cdots + \frac{1}{n} = \sum_{k=1}^{n} \frac{1}{k}.$$

Lemma 9

The sequence $s \colon \mathbb{N} \to \mathbb{R}$ with

$$s_n := H_n - \ln n$$

is monotonically decreasing and convergent. Its limit is the Euler-Mascheroni constant

$$\gamma := \lim_{n \to +\infty} (H_n - \ln n) \approx 0.5772\ldots,$$

and we have

$$\ln n < H_n - \gamma < \ln(n+1), \qquad \text{i.e.} \quad H_n \in \Theta(\ln n) = \Theta(\log n).$$

Discrete Probability: Material for Experiments

Basic elementary probability needed . . .

. . . for, e.g., analyzing randomized algorithms and data structures!

Coin:

- A coin has two sides: H (for “head”) or T (for “tail”).

Die:

- A standard die has six sides which are labelled with the numbers 1,2,3,4,5, and 6.
- Rolling a fair die will result in any of these six numbers being up.

Cards:

- A standard 52-card deck of playing cards has 13 hearts (Dt. Herz), 13 diamonds (Dt. Karo), 13 spades (Dt. Pik), and 13 clubs (Dt. Treff).
- Hearts and diamonds are red suits (Dt. Farben); spades and clubs are black suits.
- For each suit, there is a 2, 3, 4, 5, 6, 7, 8, 9, 10, jack, queen, king, and ace. Jacks, queens, and kings are so-called “face” cards.

Discrete Probability

- A *trial* is one instance of an experiment like rolling a fair die, flipping a coin or pulling a card from decently shuffled deck.

Definition 10 (*Sample space, Dt.: Ergebnisraum*)

A sample space Ω is a non-empty, finite or countably infinite set. Each element of Ω is called an *outcome* (aka elementary event, Dt.: Elementarereignis), and each subset of Ω is called an *event*.

Definition 11 (*Probability measure, Dt.: Wahrscheinlichkeit(sfunktion)*)

A probability measure $\mathrm{Pr}\colon \mathcal{P}(\Omega) \to \mathbb{R}$ is a mapping from the power set $\mathcal{P}(\Omega)$ to $\mathbb{R}$ with the following properties:

- $0 \leq \mathrm{Pr}(A) \leq 1$ for all $A \subseteq \Omega$,
- $\sum_{\omega \in S} \mathrm{Pr}(\omega) = 1$.

- This implies $\mathrm{Pr}\left(\sum_{n\in\mathbb{N}} A_n\right) = \sum_{n\in\mathbb{N}} \mathrm{Pr}(A_n)$ for every sequence $A_1, A_2, \ldots$ of pairwise disjoint sets from $\mathcal{P}(\Omega)$.

Discrete Probability Space

Definition 12 (*Discrete probability space, Dt.: diskreter Wahrscheinlichkeitsraum*)

A *(discrete) probability space* is a pair $(\Omega, \Pr)$ where Ω is a sample space and $\Pr$ is a probability measure on Ω.

- The probability of an event $A \subset \Omega$ is defined as the sum of the probabilities of the outcomes of A: $\Pr(A) := \sum_{\omega \in A} \Pr(\omega)$.
- Other common ways to denote the probability of A are $\Pr[A]$ and $\mathrm{P}(A)$ and $p(A)$.
- In the language of random experiments we understand $\Pr(A)$ for $A \subset \Omega$ as follows:

$$\Pr(A) = \frac{\text{number of outcomes favorable to } A}{\text{total number of possible outcomes}}$$

Definition 13 (*Uniform probability space*)

A probability space $(\Omega, \Pr)$ is *uniform* if Ω is finite and if for every $\omega \in \Omega$

$$\Pr(\omega) = \frac{1}{|\Omega|}.$$

Discrete Probability

Lemma 14

Complementarity: If A is an event that occurs with probability $\Pr(A)$, then $1 - \Pr(A)$ is the probability that A does not occur.

Sum: If $A \cap B = \emptyset$ for two events A, B, i.e., if A, B cannot occur simultaneously, then the probability $\Pr(A \cup B)$ that either of them occurs is $\Pr(A) + \Pr(B)$.

Definition 15 (*Conditional probability, Dt.: bedingte Wahrscheinlichkeit*)

The *conditional probability* of A given B, denoted by $\Pr(A \mid B)$, is the probability that the event A occurs given that the event B has occurred:

$$\Pr(A \mid B) = \frac{\Pr(A \cap B)}{\Pr(B)}$$

Discrete Probability

Definition 16 (*Independent Events*)

If $\Pr(B) > 0$ then event A is independent of event B if and only if

$$\Pr(A \mid B) = \Pr(A).$$

Caveat

Disjoint events are not independent! If $A \cap B = \emptyset$, then knowing that event B happened means that you know that A cannot happen!

Lemma 17

Two events A, B are independent if and only if either of the following statements is true:

$$\Pr(A) \cdot \Pr(B) = \Pr(A \cap B) \qquad \Pr(A \mid B) = \Pr(A) \qquad \Pr(B \mid A) = \Pr(B)$$

- If any one of these statements is true, then all three statements are true.

Discrete Probability: W.H.P.

Definition 18 (*With high probability*)

For $n \in \mathbb{N}$, an event A_n occurs *with high probability* if its probability depends on an integer n and goes to 1 as n goes to infinity.

- Typical example:

$$\Pr(A_n) = \left(1 - \frac{1}{n^c}\right) \quad \text{for some} \quad c \in \mathbb{R}^+.$$

- The term “with high probability” is commonly abbreviated as w.h.p. or WHP.

Random Variable

Definition 19 (*Random variable, Dt.: Zufallsvariable*)

A *random variable* X on a sample space Ω is a function $X\colon \Omega \to \mathbb{R}$ that maps each outcome of Ω to a real number. A random variable is *discrete* if it has a finite or countably infinite set of distinct possible values; it is *continuous* otherwise. It is called an *indicator random variable* if $X(\Omega) = \{0, 1\}$.

Misleading terminology!

A random variable is neither "random" nor a "variable"!

- The notation

$$X = a$$

is a frequently used short-hand notation for denoting the set of outcomes $\omega \in \Omega$ such that $X(\omega) = a$. Hence, $X = a$ is an event.
- Similarly for $X \geq a$.

Definition 20 (*Independent random variables*)

The two random variables $X_1, X_2\colon \Omega \to \mathbb{R}$ are independent if for all x_1, x_2 the two events $X_1 = x_1$ and $X_2 = x_2$ are independent.

Probability Distribution

Definition 21 (*Probability distribution, Dt.: Wahrscheinlichkeitsverteilung*)

For a discrete random variable X on a probability space $(\Omega, \Pr)$, its *probability distribution* is the function $D \colon \mathbb{R} \to \mathbb{R}$ with

$$D(x) := \begin{cases} \Pr(X = x) & \text{if } x \in X(\Omega), \\ 0 & \text{if } x \notin X(\Omega). \end{cases}$$

It is *uniform* (Dt.: gleichverteilt) for a finite codomain $X(\Omega)$ if $D(x) = {}^1/_n$ for all $x \in X(\Omega)$, with $n := |X(\Omega)|$.

- The sum of all probabilities contained in a probability distribution needs to equal 1, and each individual probability must be between 0 and 1, inclusive.

Definition 22 (*Cumulative distribution, Dt.: kumulative Wahrscheinlichkeitsverteilung*)

For a discrete random variable X on a probability space $(\Omega, \Pr)$, its *cumulative probability distribution* is the function

$$CD \colon X(\Omega) \to \mathbb{R} \qquad \text{with} \quad CD(x) := \Pr(X \leq x).$$

Expected Value of a Random Variable

Definition 23 (*Expected value, Dt.: Erwartungswert*)

The *expected value*, $\mathbb{E}(X)$, of a discrete random variable X on a probability space $(\Omega, \Pr)$ is defined as

$$\mathbb{E}(X) := \sum_{\omega \in \Omega} X(\omega) \cdot \Pr(\omega),$$

provided that this series converges absolutely.

- That is, the sum must remain finite if all $X(\omega)$ were replaced by their absolute values $|X(\omega)|$.
- The expected value of X can be rewritten as $\mathbb{E}(X) := \sum_{x \in X(\Omega)} x \cdot \Pr(X = x)$.
- Another commonly used term to denote the expected value of X is μ_X.

Expected Value of a Random Variable

Lemma 24 (*Linearity of expectation*)

Let $a, b, c \in \mathbb{R}$ and two random variables X, Y defined over the same probability space. Then

$$\mathbb{E}[aX + bY + c] = a\,\mathbb{E}[X] + b\,\mathbb{E}[Y] + c.$$

Lemma 25 (*Markov's inequality*)

Let X be a non-negative random variable and $a \in \mathbb{R}^+$. Then the probability that X is at least as large as a is at most as large as the expectation of X divided by a:

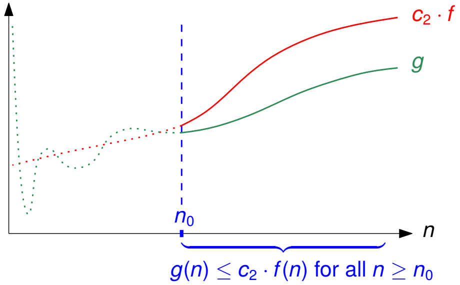
$$\Pr(X \geq a) \leq \frac{\mathbb{E}(X)}{a}.$$

Asymptotic Notation: Big-O

Definition 26 (*Big-O, Dt.: Groß-O*)

Let $f\colon \mathbb{N} \to \mathbb{R}^+$. Then the set $O(f)$ is defined as

$$O(f) \;:=\; \{g\colon \mathbb{N} \to \mathbb{R}^+ \mid \quad \exists c_2 \in \mathbb{R}^+ \quad \exists n_0 \in \mathbb{N} \quad \forall n \geq n_0 \qquad g(n) \leq c_2 \cdot f(n)\}\,.$$



- Equivalent definition used by some authors:

$$O(f) \;:=\; \left\{g\colon \mathbb{N} \to \mathbb{R}^+ \mid \quad \exists c_2 \in \mathbb{R}^+ \quad \exists n_0 \in \mathbb{N} \quad \forall n \geq n_0 \qquad \frac{g(n)}{f(n)} \leq c_2\right\}.$$

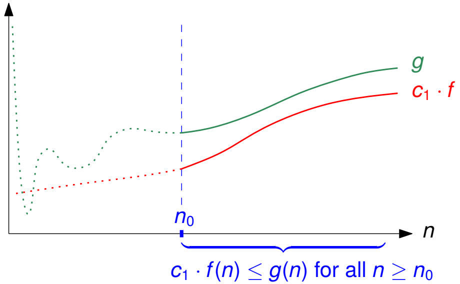
- Some authors prefer to use the symbol $\mathcal{O}$ instead of O.

Asymptotic Notation: Big-Omega

Definition 27 (*Big-Omega, Dt.: Groß-Omega*)

Let $f\colon \mathbb{N} \to \mathbb{R}^+$. Then the set $\Omega(f)$ is defined as

$$\Omega(f) := \{g\colon \mathbb{N} \to \mathbb{R}^+ \mid \exists c_1 \in \mathbb{R}^+ \quad \exists n_0 \in \mathbb{N} \quad \forall n \geq n_0 \qquad c_1 \cdot f(n) \leq g(n)\}.$$



- Equivalently,

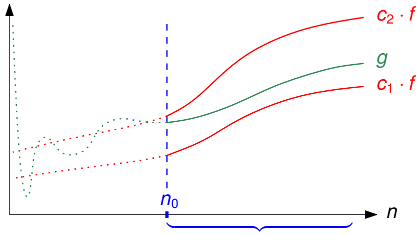
$$\Omega(f) := \left\{g\colon \mathbb{N} \to \mathbb{R}^+ \mid \exists c_1 \in \mathbb{R}^+ \quad \exists n_0 \in \mathbb{N} \quad \forall n \geq n_0 \qquad c_1 \leq \frac{g(n)}{f(n)}\right\}.$$

Asymptotic Notation: Big-Theta

Definition 28 (*Big-Theta, Dt.: Groß-Theta*)

Let $f\colon \mathbb{N} \to \mathbb{R}^+$. Then the set $\Theta(f)$ is defined as

$$\Theta(f) := \{g\colon \mathbb{N} \to \mathbb{R}^+ \mid \quad \exists c_1, c_2 \in \mathbb{R}^+ \quad \exists n_0 \in \mathbb{N} \quad \forall n \geq n_0 \quad c_1 \cdot f(n) \leq g(n) \leq c_2 \cdot f(n)\}.$$



$c_1 \cdot f(n) \leq g(n) \leq c_2 \cdot f(n)$ for all $n \geq n_0$

which is equivalent to $c_1 \leq \frac{g(n)}{f(n)} \leq c_2$ for all $n \geq n_0$

Asymptotic Notation: Small-Oh and Small-Omega

Definition 29 (*Small-Oh, Dt.: Klein-O*)

Let $f\colon \mathbb{N} \to \mathbb{R}^+$. Then the set $o(f)$ is defined as

$$o(f) := \{g\colon \mathbb{N} \to \mathbb{R}^+ \mid \quad \forall c \in \mathbb{R}^+ \quad \exists n_0 \in \mathbb{N} \quad \forall n \geq n_0 \qquad g(n) \leq c \cdot f(n)\}.$$

Definition 30 (*Small-Omega, Dt.: Klein-Omega*)

Let $f\colon \mathbb{N} \to \mathbb{R}^+$. Then the set $\omega(f)$ is defined as

$$\omega(f) := \{g\colon \mathbb{N} \to \mathbb{R}^+ \mid \quad \forall c \in \mathbb{R}^+ \quad \exists n_0 \in \mathbb{N} \quad \forall n \geq n_0 \qquad g(n) \geq c \cdot f(n)\}.$$

- We can extend Defs. 26–30 such that $\mathbb{N}_0$ rather than $\mathbb{N}$ is taken as the domain (Dt.: Definitionsmenge). We can also replace the codomain (Dt.: Zielbereich) $\mathbb{R}^+$ by $\mathbb{R}_0^+$ (or even $\mathbb{R}$) provided that all functions are eventually positive.

Warning

The use of the equality operator "$=$" instead of the set operators "$\in$" or "$\subseteq$" to denote set membership or a subset relation is a *common abuse of notation*.

Soft-Oh

Definition 31 (*Soft-Oh*)

Let $f, g\colon \mathbb{N} \to \mathbb{R}^+$. Then $g \in \tilde{O}(f)$ if and only if there exists $k \in \mathbb{N}_0$ such that $g \in O(f \log^k(f))$.

- Similarly for $\tilde{\Omega}(f)$ and $\tilde{\Theta}(f)$.

Master Theorem

Theorem 32

Consider constants $n_0 \in \mathbb{N}$ and $a \in \mathbb{N}$, $b \in \mathbb{R}$ with $b > 1$, and a function $f\colon \mathbb{N} \to \mathbb{R}_0^+$. Let $T\colon \mathbb{N} \to \mathbb{R}_0^+$ be an eventually non-decreasing function such that

$$T(n) = a \cdot T\left(\frac{n}{b}\right) + f(n)$$

for all $n \in \mathbb{N}$ with $n \geq n_0$, where we interpret $\frac{n}{b}$ as either $\lceil \frac{n}{b} \rceil$ or $\lfloor \frac{n}{b} \rfloor$. Then we have

$$T \in \begin{cases} \Theta(f) & \text{if } \begin{cases} f \in \Omega\left(n^{(\log_b a)+\varepsilon}\right) \text{ for some } \varepsilon \in \mathbb{R}^+, \\ \text{and if the following regularity condition holds} \\ \text{for some } 0 < s < 1 \text{ and all sufficiently large n:} \\ \quad a \cdot f\left({}^{n}/_{b}\right) \leq s \cdot f(n), \end{cases} \\ \Theta\left(n^{\log_b a} \log n\right) & \text{if } f \in \Theta\left(n^{\log_b a}\right), \\ \Theta(n^{\log_b a}) & \text{if } f \in O\left(n^{(\log_b a)-\varepsilon}\right) \text{ for some } \varepsilon \in \mathbb{R}^+. \end{cases}$$

- This is a simplified version of the Akra-Bazzi Theorem [Akra&Bazzi (1998)].

Basics of Algorithm Theory

“Problem”

Problem

A *problem* is the concise (abstract) description of every permissible input and of the output sought for every (permissible) input.

- E.g., we can specify the sorting problem for (real) numbers as follows:

Problem: SORTING

Input: A sequence of n (real) numbers $(x_1, x_2, \ldots, x_n)$, for some $n \in \mathbb{N}$.

Output: A permutation $\pi \in S_n$ such that $x_{\pi(1)} \leq x_{\pi(2)} \leq \ldots \leq x_{\pi(n)}$.

Problem instance

An *instance of a problem* is one particular (permissible) input.

- E.g., sorting the five numbers of the sequence $(3, 1, 5, 14, 8)$ forms one instance of the SORTING problem.
- We have $n = 5$, and SORTING these numbers requires us to find the permutation

$$\pi = \begin{pmatrix} 1 & 2 & 3 & 4 & 5 \\ 2 & 1 & 3 & 5 & 4 \end{pmatrix}.$$

“Algorithm”

Algorithm

An *algorithm* is a sequence of self-contained step-by-step instructions for solving a problem.

- The term “algorithm” is generally assumed to stem from the (Latin transliteration) of the name of a Persian mathematician who was a scholar at the House of Wisdom at Baghdad during the Abbasid Caliphate: Muḥammad ibn Mūsā al-Khwārizmī (ca. 780–850).
- An algorithm may be encoded as a procedure, a formula, a recipe, . . .
- Attempts to formalize the concept of an algorithm started with work on the Entscheidungsproblem (posed by Hilbert in 1928). Formalizations include
    - the theory of recursive functions [Gödel, Herbrand, Kleene (1930–1935)],
    - lambda calculus [Church (1936)],
    - Turing machines [Turing (1936–1939)].
- See a textbook on theoretical computer science for formal foundations of “algorithm”.
- In this lecture we will presuppose a general understanding of “algorithm” and use English language, pseudocode or C/C++ as algorithmic notations.

Decision Problem

Definition 33 (*Decision Problem; Dt.: Entscheidungsproblem*)

A problem is a *decision problem* if the output sought for a particular instance of the problem always is the answer *yes* or *no*.

- Famous decision problem: Boolean satisfiability (SAT).

Problem: SAT

Input: A propositional formula A.

Decide: Is A satisfiable? I.e., does there exist an assignment of truth values to the Boolean variables of A such that A evaluates to true?

- Note that a solution to SAT does not necessarily require us to know suitable truth assignments to the Boolean variables.
- However, if we are given truth assignments for which A is claimed to evaluate to true then this claim is easy to verify.
- We'll get back to this issue when talking about $\mathcal{NP}$-completeness ...

Decision Problem vs. Computational/Optimization Problems

- Often a decision problem is closely related to an underlying computational/optimization problem.
  E.g., “Sort the numbers $x_1, \dots, x_n$” versus “Are the numbers $x_1, \dots, x_n$ sorted?”

Problem: CHROMATICNUMBER

Input: An undirected graph $\mathcal{G}$.

Output: An assignment of colors to the nodes of $\mathcal{G}$ such that no neighboring nodes bear the same color and such that a minimum number of colors is used.

Problem: *k*-COL

Input: An undirected graph $\mathcal{G}$ and a constant $k \in \mathbb{N}$ with $k > 3$.

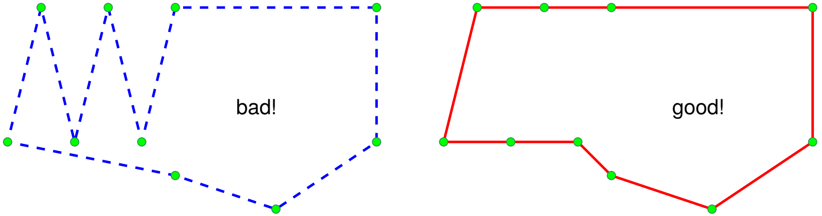
Decide: Do k colors suffice to color the nodes of $\mathcal{G}$ such that no neighboring nodes bear the same color?

Decision Problem vs. Computational/Optimization Problems

Problem: EUCLIDEANTRAVELINGSALESMANPROBLEM (ETSP)

Input: A set S of n points in the Euclidean plane.

Output: A cycle of minimum length that starts and ends in one point and visits all points of S.



Problem: EUCLIDEANTRAVELINGSALESMANPROBLEM — DECISION

Input: A set S of n points in the (Euclidean) plane and a constant $c \in \mathbb{R}^+$.

Decide: Does there exist a cycle that starts and ends in one point and visits all points of S such that the length of that cycle is less than c?

Inverse Ackermann

Definition 34 (*Inverse Ackermann function*)

For $m, n \in \mathbb{N}_0$, the *Ackermann function* is defined as follows [Péter (1935)]:

$$A(m,n) := \begin{cases} n+1 & \text{if } m = 0, \\ A(m-1,1) & \text{if } m > 0 \text{ and } n = 0, \\ A(m-1, A(m, n-1)) & \text{if } m > 0 \text{ and } n > 0. \end{cases}$$

The *inverse Ackermann function* is given by

$$\alpha(n) := \min\{k \in \mathbb{N} : A(k,k) \geq n\}.$$

- The Ackermann function grows extremely rapidly. E.g., we have

$$A(4,4) \approx 2^{2^{2^{2^{16}}}} \approx 2^{2^{2 \cdot 10^{19728}}}.$$

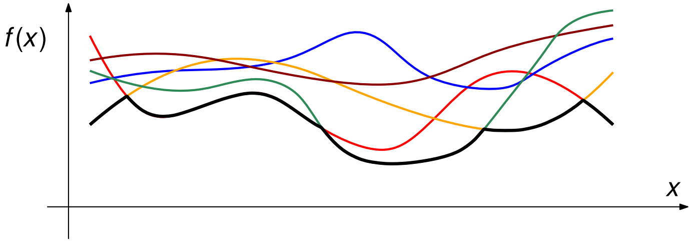
- Hence, the inverse Ackermann function grows extremely slowly; it is at most four for any input of practical relevance.
- But it does grow unboundedly as n grows, and we have $1 \in o(\alpha)$!
- Real-world occurrence of $O(\alpha)$: Combinatorial complexity of lower envelopes.

Inverse Ackermann and Lower Envelopes

Definition 35 (*Lower envelope, Dt.: untere Hüllkurve*)

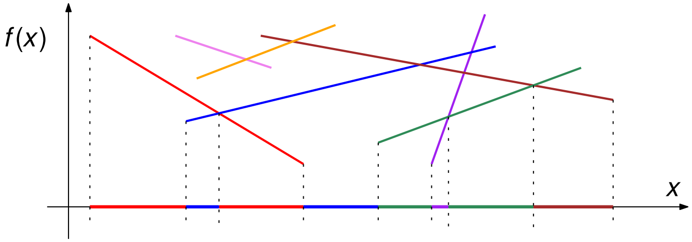
Consider a set of n real-valued functions $f_1, f_2, \ldots, f_n$ over the same domain. Their *lower envelope* is the function $f_{\min}$ given by the pointwise minimum of $f_1, f_2, \ldots, f_n$:

$$f_{\min}(x) := \min\{f_i(x) \colon 1 \le i \le n\}.$$



Inverse Ackermann and Lower Envelopes

- The concept of a lower envelope can be extended naturally to a set of partially defined functions over the same domain.
- In particular, it extends to straight-line segments in the plane.
- The projection of the lower envelope onto the x-axis gives a sequence of intervals, and the theory of Davenport-Schinzel sequences implies the following result [Sharir&Agarwal (1995)]: The lower envelope of n line segments contains at most $\Theta(n\,\alpha(n))$ segments and vertices — and this bound is tight!



Log-star

Definition 36 (*Iterated logarithm*)

For $x \in \mathbb{R}^+$ the *iterated logarithm* (aka *log-star*) is defined as follows:

$$\log^* x := \begin{cases} 0 & \text{if } x \leq 1, \\ 1 + \log^*(\log x) & \text{if } x > 1. \end{cases}$$

- E.g., for the binary logarithm, $\log 65\,536 = \log 2^{16} = 16$ but (since $2^{16} = 2^{2^{2^2}}$)
$$\log^* 2^{16} \overset{\text{def}}{=} 1 + \log^* 2^{2^2} \overset{\text{def}}{=} 2 + \log^* 2^2 \overset{\text{def}}{=} 3 + \log^* 2^1 \overset{\text{def}}{=} 4 + \log^* 1 \overset{\text{def}}{=} 4.$$
- Log-star grows very slowly. It is at most six for any input of practical relevance: We have
$$2^{65536} = 2^{2^{16}} \approx 2 \cdot 10^{19728}, \quad \text{with } \log^* 2^{65536} = 5.$$
- We have $\alpha \in o(\log^*)$.
- Log-star shows up in the complexity bound of Fürer's algorithm [2007] for multiplying large integers: If n denotes the total number of bits of the two input numbers then an optimized version of his algorithm runs in time $O(n \log n\, 2^{3\log^* n})$ [Harvey et al. (2014)]. For truly large values of n this is slightly better then the $O(n \log n \log\log n)$ bound of the Schönhage-Strassen algorithm [1971].

Logarithmic Growth

- Recall Lemma 3:

$$\log_\alpha(n) = \frac{1}{\log_\beta(\alpha)} \cdot \log_\beta(n) \quad \text{for all } \alpha, \beta \in \mathbb{R}^+ \setminus \{1\} \text{ and all } n \in \mathbb{N}.$$

  Hence,

$$\Theta(\log_\alpha n) = \Theta(\log_\beta n) \quad \text{for all } \alpha, \beta \in \mathbb{R}^+ \setminus \{1\}.$$

- Note that Stirling's formula asserts

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n, \qquad \text{thus, } \Theta(\log n!) = \Theta(n \log n).$$

- Recall Lemma 9. Since

$$\lim_{n \to +\infty} (H_n - \ln n) = \gamma,$$

  we know that

$$\sum_{k=1}^{n} \frac{1}{k} = \Theta(\ln n) = \Theta(\log n).$$

Polylogarithmic

Definition 37 (*Polylogarithmic*)

An algorithm runs in *polylogarithmic* time if

$$T \in O(\log^k) \quad \text{for some constant } k \in \mathbb{N}$$

holds for its time complexity T.

- This is also written as $O(\text{poly}(\log n))$.
- Often abbreviated as "polylog".
- Polylog times are examples for *sublinear* times.

Quasilinear Time

Definition 38 (*Quasilinear*)

An algorithm runs in *quasilinear* time if

$$T \in O(n \log^k n) \quad \text{for some constant } k \in \mathbb{N}$$

holds for its time complexity T.

- This is also written as $O(n\,\mathrm{poly}(\log n))$.
- Using soft O-notation, quasilinear time may be written as $\tilde{O}(n)$.

(Quasi-)Polynomial Time

Definition 39 (*Polynomial*)

An algorithm runs in *polynomial* time if

$$T \in O(n^k) \quad \text{for some constant } k \in \mathbb{N}$$

holds for its time complexity T.

- This is also written as $O(\mathrm{poly}(n))$.

Definition 40 (*Quasi-polynomial*)

An algorithm runs in *quasi-polynomial* time if

$$T \in 2^{O(\log^c n)} \quad \text{for some constant } c > 1$$

holds for its time complexity T.

- For $c := 1$ we get a polynomial-time algorithm, and for $c < 1$ we get a sublinear algorithm.

Exponential Time

Definition 41 (*Exponential*)

An algorithm runs in *exponential* time if

$$T \in O(2^{n^k}) \quad \text{for some constant } k \in \mathbb{N}$$

holds for its time complexity T.

- This is also written as $O(2^{\text{poly}(n)})$.
- Note: Some authors require $T \in 2^{O(n)}$.

Factorial and Double Exponential Time

Definition 42 (*Factorial*)

An algorithm runs in *factorial* time if

$$T \in O(n!)$$

holds for its time complexity T.

- We have $2^n \in o(n!)$ and $n! \in o(2^{n^{1+c}})$ for all $c > 0$.

Definition 43 (*Double Exponential*)

An algorithm runs in *double exponential* time if

$$T \in O(2^{2^{n^k}}) \quad \text{for some constant } k \in \mathbb{N}$$

holds for its time complexity T.

Comparison of Growth Rates

n	$\log n$	$\log\log n$	$\log^* n$	$\alpha(n)$
2	1	0	1	1
2^2	2	1	2	2
$2^{2^2} = 16$	4	2	3	3
$2^{16} = 65\,536$	16	4	4	4
$2^{64} \approx 1.8 \cdot 10^{19}$	64	6	5	4
$2^{2^{2^{2^{16}}}}$	$2^{2^{2^{16}}}$	$2^{2^{16}}$	7	4
$\underbrace{2^{2^{2^{\cdot^{\cdot^{\cdot^{2}}}}}}}_{2023}$	$\underbrace{2^{2^{\cdot^{\cdot^{\cdot^{2}}}}}}_{2022}$	$\underbrace{2^{2^{\cdot^{\cdot^{\cdot^{2}}}}}}_{2021}$	2023	4
?				5

The Expression $k + \varepsilon$

- A statement of the form "$k + \varepsilon$ for any positive $\varepsilon \in \mathbb{R}$" means that some claim holds no matter which positive constant $\varepsilon \in \mathbb{R}^+$ is added to k.
- The constant ε may be regarded as arbitrarily small but it will never equal zero.
- E.g., suppose that some algorithm runs in $2^c n^{1+1/c}$ time, where $c \in \mathbb{R}^+$ is a user-chosen constant:
  - For $c := 2$, the complexity term equals $4n^{3/2}$, which is in $O(n^{3/2})$.
  - For $c := 9$, the complexity term equals $2^9 n^{10/9}$, which is in $O(n^{10/9})$.
  - It is easy to see that $1 + {}^1\!/c$ approaches 1 as c approaches infinity.
  - However, c cannot be set to infinity (or made arbitrarily large) since then the 2^c term would dominate the complexity of our algorithm.
  - Hence, this complexity is best expressed as "$O(n^{1+\varepsilon})$ for any positive ε".
- In a nutshell, $O(n^{k+\varepsilon})$ means that the upper bound is of the form $c_\varepsilon \cdot n^k \cdot n^\varepsilon$, for any $\varepsilon \in \mathbb{R}^+$, where the constant c_ε depends on ε. Typically, c_ε grows unboundedly as ε goes to zero.

Complexity of an Algorithm

- Typical kinds of complexities studied:
  - time complexity, i.e., a mathematical assessment or estimation of the running time independent of a particular implementation or platform;
  - space complexity, i.e., a mathematical assessment or estimation of the number of memory units consumed by the algorithm;
  - complexity of the output generated.

Definition 44 (*Worst-Case Complexity, Dt.: Komplexität im schlimmsten Fall*)

A *worst-case complexity* of an algorithm is a function $f\colon \mathbb{N} \to \mathbb{R}^+$ that gives an upper bound on the number of elementary operations (memory units, ...) used by an algorithm with respect to the size of its input, for all inputs of the same size.

Definition 45 (*Average-Case Complexity, Dt.: Komplexität im durchschnittl. Fall*)

An *average-case complexity* of an algorithm is a function $g\colon \mathbb{N} \to \mathbb{R}^+$ that models the average number of elementary operations (memory units, ...) used by an algorithm with respect to the size of its input.

- So, what does “size of its input” mean? And what are “elementary operations”?

Input Size

Definition 46 (*Input Size, Dt.: Eingabegröße*)

The *size of the input* of an algorithm is a quantity that measures the number of input items relevant for elementary operations of the algorithm.

- For most problems the choice of an appropriate measure of the input size will be fairly obvious.
- E.g., for sorting a typical measure of the input size will be the number of records to be sorted (if constant memory and comparison time per record may be assumed).
- If we are to check for intersections among line segments then it seems natural to take the number of line segments as input size.
- A graphics rendering application may want to consider the number of triangles to be rendered as input size.

Input Size — It Does Matter!

Problem: PRIME

Input: A natural number n with $n > 1$.

Decide: Is n prime? I.e., can n be divided only by 1 and by itself?

```
boolean IsPrime(int n)
{
   for (j := 2;  j <= sqrt(n);  j++) {
      if ( (n mod j) == 0 )  return false;
   };
   return true;
}
```

- Complexity:
  - The body of the loop is executed $O(\sqrt{n})$ times.
  - If the operation ($n \mod j$) can be implemented to run in $O(n)$ time, then this algorithm solves problem PRIME in $O(n\sqrt{n})$ steps!?

Input Size — It Does Matter!

- However: What is the input size? Does the description of a number n really require $O(n)$ characters?
  - In the decimal system: $\textsc{Size}_{10}(1000) = 4$.
  - In the dual system: $\textsc{Size}_{2}(1000) \approx 10$.
  - Thus, in the dual system, an input of size k results in $O((2^k)^{3/2})$ many steps being carried out by our simple algorithm!
  - Note: The latter bound is exponential in k!

Model of Computation

- We continue with (informal!) definitions that pertain to the complexity analysis of algorithms.

Definition 47 (*Elementary Operation, Dt.: Elementaroperation*)

An *elementary operation* is an operation whose running time is assumed not to depend on the specific values of its operands.

- E.g., the time taken by the comparison of two floating-point numbers is frequently assumed to be constant.
- Still, what constitutes an elementary operation depends on the model of computation.

Definition 48 (*Model of Computation*)

A *model of computation* specifies the elementary operations that may be executed, together with their respective costs.

Model of Computation

- Purely theoretical point of view: Turing Machine (TM) model.
- This is the model to use when talking about theoretical issues like $\mathcal{NP}$-completeness!
- But the TM model is cumbersome to use for analyzing actual complexities and, thus, is impractical for most "real" applications . . .
- Hence several alternative models have been proposed, e.g.:
    - Random Access Machine (RAM) model,
    - Word RAM model,
    - Real RAM model,
    - Blum-Shub-Smale model,
    - Algebraic Decision/Computation Tree (ADT/ACT) model.

Warning

While all these models are "good enough from a practical point of view" to shed some light on the complexity of an algorithm or a problem, they do differ in detail. Different models of computation are not equally powerful, and complexity results need not transfer readily from one model to another model.

- Consult a textbook on theoretical computer science for details . . .

Algebraic Computation Tree

Definition 49 (*Algebraic computation tree, Dt.: algebr. Berechnungsbaum*)

An *algebraic computation tree* with input $(x_1, x_2, \ldots, x_n) \in \mathbb{R}^n$ solves a decision problem P if it is a finite rooted tree with at most two children per node and two types of internal nodes:

Computation: A computation node v has a value f_v determined by one of the following instructions:

$$f_v = f_u \circ f_w \quad \text{or} \quad f_v = \sqrt{f_u}$$

where $\circ \in \{+, -, \cdot, /\}$ and f_u, f_w are values associated with ancestors of v, input variables or arbitrary real constants.

Branch: A branch node v has two children and contains one of the predicates

$$f_u > 0 \qquad f_u \geq 0 \qquad f_u = 0$$

where f_u is a value associated with an ancestor of v or an input variable.

Every leaf node is associated with *Yes* and *No*, depending on the correct answer for every $(x_1, x_2, \ldots, x_n)$ relative to P.

Membership Set

- Of course, we require that no computation node leads to a division by zero or to taking the square root of a negative number.

Definition 50 (*Membership set*)

For a decision problem P with input variables $x_1, x_2 \dots, x_n \in \mathbb{R}$ we define W_P as the set of points in $\mathbb{R}^n$ for which the answer to the decision problem is *Yes*:

$$W_P := \{(u_1, \dots, u_n) \in \mathbb{R}^n : u_1, u_2 \dots, u_n \text{ yield "}\textit{Yes}\text{" for } P\}.$$

The set W_P is called the *membership set* of P.
Also: $\overline{W_P} := \mathbb{R}^n \setminus W_P$.

- Thus, $\overline{W_P}$ contains the points in $\mathbb{R}^n$ for which the answer is *No*.

Definition 51

For a decision problem P with input $x_1, x_2 \dots, x_n \in \mathbb{R}$ and membership set W_P we denote the number of disjoint connected components of W_P by $\#(W_P)$, and the number of disjoint connected components of $\overline{W_P}$ by $\#(\overline{W_P})$.

Algebraic Computation Trees and Lower Bounds

Theorem 52

If we exclude all intermediate nodes which correspond to additions, subtractions and multiplications by constants then we get for the height h of an algebraic computation tree that solves a decision problem P:

$$h = \Omega(\log(\#(W_P) + \#(\overline{W_P})) - n).$$

- Theorem 52 is a consequence of a clever adaption by Steele&Yao [1982] and Ben-Or [1983] of a classical result in algebraic geometry obtained independently by Petrovskiĭ&Oleĭnik [1952], Milnor [1964] and Thom [1965].
- For fixed-dimensional input, the real RAM model and the ACT model are equivalent.

Reduction of a Problem: Humorous View of Reductions

Difference between a mathematician and an engineer?

One can perform the following experiment to tell the difference between a mathematician (or theoretical computer scientist) and an engineer:

1. Put an empty kettle in the middle of the kitchen floor and tell your subjects to boil some water.
   - The engineer will fill the kettle with water, put it on the (electric) stove, and turn the electricity on.
   - The mathematician will proceed similarly.
2. Next, put the kettle already filled with water on the stove, and ask the subjects to boil the water.
   - The engineer will turn the electricity on and boil the water.
   - The mathematician will empty the kettle and put it in the middle of the kitchen floor — and claim the problem to be solved by having it reduced to a problem whose solution is already known!

Reduction of a Problem

Definition 53 (*Reduction*)

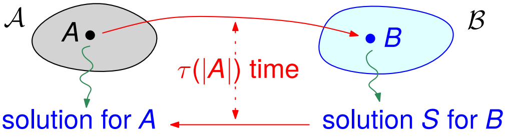
A problem $\mathcal{A}$ can be *reduced* (or *transformed*) to a problem $\mathcal{B}$ if

1. every instance A of $\mathcal{A}$ can be converted to an instance B of $\mathcal{B}$,
2. a solution S for B can be computed, and
3. S can be transformed back into a correct solution for A.

Definition 54

A problem $\mathcal{A}$ is τ-*reducible* to $\mathcal{B}$, denoted by $\mathcal{A} \leq_\tau \mathcal{B}$, if

1. $\mathcal{A}$ can be reduced to $\mathcal{B}$,
2. for any instance A of $\mathcal{A}$, steps 1 and 3 of the reduction can be carried out in at most $\tau(|A|)$ time, where $|A|$ denotes the input size of A.



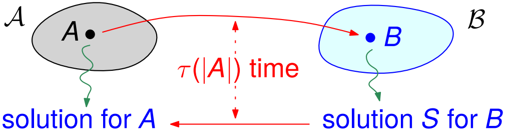
Transfer of Complexity Bounds

Lemma 55 (*Upper bound via reduction*)

Suppose that $\mathcal{A}$ is τ-reducible to $\mathcal{B}$ such that the order of the input size is preserved. If problem $\mathcal{B}$ can be solved in $O(T)$ time, then $\mathcal{A}$ can be solved in at most $O(T + \tau)$ time.

Lemma 56 (*Lower bound via reduction*)

Suppose that $\mathcal{A}$ is τ-reducible to $\mathcal{B}$ such that the order of the input size is preserved. If problem $\mathcal{A}$ is known to require $\Omega(T)$ time, then $\mathcal{B}$ requires at least $\Omega(T - \tau)$ time.



Transfer of Time Bounds: SORTING and ELEMENTUNIQUENESS

Problem: ELEMENTUNIQUENESS

Input: A set S of n real numbers $x_1, x_2, \dots, x_n$.

Decide: Are any two numbers of S equal?

- Obviously, after sorting $x_1, x_2, \dots, x_n$ we can solve ELEMENTUNIQUENESS in $O(n)$ time.
- Hence, reduction yields the following result:

Lemma 57

- ELEMENTUNIQUENESS can be solved in time $O(f) + O(n)$ if we can sort n numbers in $O(f)$ time, for some $f: \mathbb{N} \to \mathbb{R}^+$.
- SORTING requires $\Omega(f)$ time if ELEMENTUNIQUENESS requires $\Omega(f)$ time, for some $f: \mathbb{N} \to \mathbb{R}^+$ with $\lambda n.n \in o(f)$.

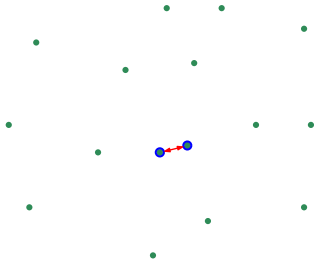
Transfer of Time Bounds: ClosestPair and ElementUniqueness

Problem: ClosestPair

Input: A set S of n points in the Euclidean plane.

Output: Those two points of S whose mutual distance is minimum among all pairs of points of S.

- We allow points to coincide but still expect them to be distinguishable by some additional data associated with each point. E.g., by means of their indices.



Transfer of Time Bounds: CLOSESTPAIR and ELEMENTUNIQUENESS

Lemma 58

1. ELEMENTUNIQUENESS can be solved in $O(f) + O(n)$ time if CLOSESTPAIR can be solved in $O(f)$ time.
2. CLOSESTPAIR requires $\Omega(f)$ time if ELEMENTUNIQUENESS requires $\Omega(f)$ time (and if $\lambda n.n \in o(f)$).

Proof :

- We reduce ELEMENTUNIQUENESS to CLOSESTPAIR.
- Let $S' := \{x_1, x_2, ..., x_n\} \subset \mathbb{R}$ be an instance of ELEMENTUNIQUENESS.
- We transform S' into an instance of CLOSESTPAIR by mapping each real number x_i to the point $(x_i, 0) \in \mathbb{R}^2$. All points of the resulting set S of points lie on the x-axis.
- Obviously, all elements of S' are unique if and only if the closest pair of S has a non-zero distance.
- It is also obvious that these transformations are carried out in $O(n)$ time.
- Hence, we get a lower bound on the time complexity of CLOSESTPAIR and an upper bound on the time complexity of ELEMENTUNIQUENESS.

$\square$

Transfer of Time Bounds: SORTING and CONVEXHULL

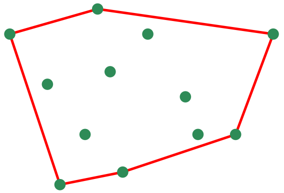
Definition 59 (*Convex set*)

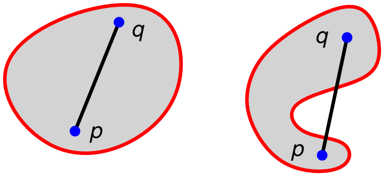
A set $X \subset \mathbb{R}^2$ is *convex* if for every pair of points $p, q \in X$ also the line segment $\overline{pq}$ is contained in X.

Problem: CONVEXHULL

Input: A set S of n points in the Euclidean plane $\mathbb{R}^2$.

Output: The convex hull $CH(S)$, i.e., the smallest convex super set of S.





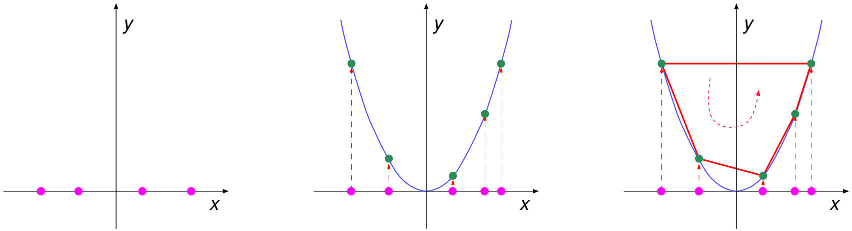
convex not convex

Transfer of Time Bounds: SORTING and CONVEXHULL

Lemma 60

> CONVEXHULL requires $\Omega(f)$ time if SORTING requires $\Omega(f)$ time, for some $f\colon \mathbb{N} \to \mathbb{R}^+$ with $\lambda n.n \in o(f)$.

- Suppose that the instance of SORTING is the set $S' := \{x_1, x_2, ..., x_n\} \subset \mathbb{R}$.
- We transform S' into an instance of CONVEXHULL by mapping each real number x_i to the point $(x_i, {x_i}^2)$. All points of the resulting set S of points lie on the parabola $y = x^2$.
- One pass along $CH(S)$ will find the smallest element. The sorted numbers can be obtained by a second pass through this list, at a total extra cost of $O(n)$ time.



Lower Bound for ElementUniqueness

- What is a lower bound on the number of comparisons for ElementUniqueness?
- We investigate our problem for $n := 3$:

$$\begin{array}{lllll} x_1 < x_2 < x_3 & \qquad & x_2 < x_3 < x_1 \\ x_1 < x_3 < x_2 & & x_3 < x_1 < x_2 \\ x_2 < x_1 < x_3 & & x_3 < x_2 < x_1 \end{array}$$

  If and only if one of these inequalities is true, then all numbers are different, and the answer to our decision problem is *No*.
- We define the subset $\overline{W_P}$ of $\mathbb{R}^3$ for which the answer is *No*:

$$\overline{W_P} := \bigcup_{\pi \in S_3} \overline{W_\pi}$$

  with

$$\overline{W_\pi} := \{(x_1, x_2, x_3) \in \mathbb{R}^3 : \quad x_{\pi(1)} < x_{\pi(2)} < x_{\pi(3)}\}.$$

- We get $\#(\overline{W_P}) = 6$ because each permutation π results in its own connected component (that is disjoint from all other components of $\overline{W_P}$).

Lower Bound for ElementUniqueness

- For $\mathbb{R}^n$ we have $\#(\overline{W_P}) = n\,!$:
  - Let $\pi, \sigma \in S_n$ with $\pi \neq \sigma$. For $1 \leq i, j \leq n$ we define
  $$f_{ij}(x_1, x_2, \ldots, x_n) := x_i - x_j.$$
  - All these functions are continuous and have a constant sign on $\overline{W_\pi}$ and $\overline{W_\sigma}$.
  - Since $\pi \neq \sigma$, there exist $i \neq j$ such that
  $$f_{ij}(p) > 0 \quad \text{for all } p \in \overline{W_\pi} \quad \text{but} \quad f_{ij}(p) < 0 \quad \text{for all } p \in \overline{W_\sigma}.$$
  - By the intermediate value theorem of calculus, any path from a point in $\overline{W_\pi}$ to a point in $\overline{W_\sigma}$ must pass through a point q where $f_{ij}(q) = 0$.
  - But $q \notin \overline{W_P}$.
  - Hence, $\overline{W_\pi}$ and $\overline{W_\sigma}$ lie in two different connected components if $\pi \neq \sigma$.
  - Since $|S_n| = n!$, we know that $\#(\overline{W_P}) \geq n!$.
- Based on Theorem 52, we conclude that the height h of an ACT is
$$h = \Omega(\log(n!) - n),$$
i.e., that $\Omega(\log n\,!) = \Omega(n \log n)$ comparisons are necessary (in the worst case) to solve ElementUniqueness in any ACT for n input numbers.

Lower Bound for ElementUniqueness

Theorem 61

A (comparison-based) solution of ElementUniqueness for n real numbers requires $\Omega(n \log n)$ comparisons in the worst case.

Corollary 62

A (comparison-based) Sorting of n real numbers requires $\Omega(n \log n)$ comparisons.

- Comparison-based sorting means that the sorted order is achieved only by using comparisons among the input elements (relative to a total order on them).

Corollary 63

A solution to ConvexHull for n points requires $\Omega(n \log n)$ time in the ACT model in the worst case.

Corollary 64

A solution to ClosestPair for n points requires $\Omega(n \log n)$ time in the ACT model in the worst case.

Adversary Strategy

- Can we come up with a "model" of the worst case?
- For some problems the answer is "yes", by employing an *adversary strategy*.
- Two players, A and B, play the following game: A thinks of n distinct real numbers, and B tries to sort those numbers by comparing pairs of two numbers.
- Of course, B does not know (the order of) A's numbers.
- Comparisons: B is allowed to ask questions of the form "Is your third number greater than your fifth number?"
- No cheating! A has to answer truthfully and consistently.
- Note, however, that A can replace his originally chosen n numbers by a new n-tuple of numbers, at any time during the game, provided that the new numbers are consistent with the answers that A has given so far.
- In particular, if this does not contradict answers given so far, then A can re-order his numbers at any time during the game at his discretion.
- What is a lower bound on the number of comparisons that A can force B to make?
- Player A uses an adversary strategy to prove that $\Omega(n \log n)$ constitutes a lower bound for the number of comparisons which B has to make in the worst case, i.e., to the number of steps that it takes B to sort those n numbers.
- There are $n!$ different permutations. Thus, player B (sorting algorithm) must decide among $n!$ different sequences of comparisons to identify the order of the numbers.

Adversary Strategy: Lower Bound for Sorting

- We assume that A stores the n numbers in an array $a[1, \ldots, n]$, and that B will sort the numbers by comparing some element $a[i]$ to some other element $a[j]$, i.e., by asking A whether $a[i] < a[j]$.
- Since the adversary A is allowed to pick the input, the adversary A keeps a set S of permutations that are consistent with the comparisons B has made so far.
- The answer of A to a comparison “Is $a[i] < a[j]$?” is chosen as follows:
  - Let $Y \subset S$ be those permutations that have remained in S and that are also consistent with $a[i] < a[j]$.
  - Furthermore, $N := S \setminus Y$.
  - If $|Y| \geq |N|$ then the adversary A prefers to answer “yes” and then replaces S by Y.
  - Otherwise, “no” is answered and S is replaced by N.
- This strategy allows A to keep at least half of the permutations after every comparison of the algorithm B.
- Player B cannot declare the order of the numbers to be known (and, thus, the numbers to be sorted) as long as $|S| > 1$.
- Thus, B needs at least $\Omega(\log(n!)) = \Omega(n \log n)$ comparisons, which establishes the lower bound sought.

Amortized Analysis: Motivation

- Amortized analysis is a worst-case analysis of a sequence of different operations performed on a datastructure or by an algorithm.
- It is applied if a costly operation cannot occur for a series of operations in a row.
- With traditional worst-case analysis, the resulting bound on the running time of such a sequence of operations is too pessimistic if the execution of a costly operation can only happen after many cheap operations have already been carried out.
- The goal of amortized analysis is to obtain a bound on the overall cost of a sequence of operations or the average cost per operation in the sequence which is tighter than what can be obtained by separately analyzing each operation in the sequence.
- Introduced in the mid 1970s to early 1980s, and popularized by Tarjan in “Amortized Computational Complexity” [Tarjan (1985)].
- Finance: Amortization refers to paying off a debt by smaller payments made over time.

Amortized Analysis: Dynamic Array

- A *dynamic array* is a data structure of variable size that allows to store and retrieve elements in a random-access mode.
- Elements can also be inserted at and deleted from the end of the array.
- To be distinguished from a dynamically allocated array, which is an array whose capacity is fixed at the time when the array is allocated.
- Simple realization of a dynamic array: Use a dynamically allocated array of fixed size and reallocate whenever needed to increase (or decrease) the capacity of the array.
  - Size: Number of contiguous elements stored in the dynamic array.
  - Capacity: Physical size of the underlying fixed-sized array.

  Insertion of an element at the end of the array:
  - Constant-time operation if the size is less than the capacity.
  - Costly if the dynamic array needs to be resized since this involves allocating a new underlying array and copying each element from the original array.
- How shall we resize the dynamic array?

Amortized Analysis: Dynamic Array

- Suppose that the initial capacity of the array is 1.
- Simple strategy: We increase the capacity by one whenever the size of the array gets larger than its capacity.
- In the worst case, a sequence of n array operations consists of only insertions at the end of the array, at a cost of k for the insertion of the k-th element into an array of size $k-1$.
- Hence, we get $1+2+\ldots+n = \frac{n(n+1)}{2} \in O(n^2)$ as total worst-case complexity for n insert operations, i.e., $O(n)$ per operation.
- Can we do better?

```
AddAtEndOfArray(dynamicArray A, element e) {
   if (A.size == A.capacity) {
      A.capacity += 1;
      copy contents of A to new memory location;
   }
   A[A.size] = e;
   A.size += 1;
}
```

Amortized Analysis: Dynamic Array

- To avoid the costs of frequent resizing we expand the array by a constant factor α whenever we run out of space. E.g., we can double its capacity.
- Amortized analysis allows to show that the (amortized) cost per array operation is reduced to $O(1)$.
- Amortized constant cost per operation is achieved for any growth factor $\alpha > 1$.
  - C++: `std::vector` with $\alpha := 2$ for GCC/Clang, and $\alpha := \frac{3}{2}$ for MS VC++.
  - Java: `ArrayList` with $\alpha := \frac{3}{2}$.

  The best value for the growth factor α is a topic of frequent discussions.
- Could also shrink the array if its size falls below some percentage of its capacity.

```
InsertIntoArray(dynamicArray A, element e) {
   if (A.size == A.capacity) {
      A.capacity *= 2;
      copy contents to new memory location;
   }
   A[A.size] = e;
   A.size += 1;
}
```

Amortized Analysis: Basics

Definition 65 (*Amortized cost*)

The *amortized cost* of one operation out of a permissible sequence of n operations, for some $n \in \mathbb{N}$, is the total (worst-case) cost for all operations divided by n.

- Amortized analysis
  - does not depend on a particularly "good" sequence of operations;
  - considers arbitrary sequences, and, in particular, worst-case sequences;
  - gives genuine upper bounds: the amortized cost per operation times the number of operations yields a worst-case bound on the total complexity of any permissible sequence of those operations;
  - guarantees the average performance of each operation in the worst case;
  - does not involve probabilities;
  - averages over time.
- Average-case analysis
  - averages over the input;
  - typically depends on assumptions on probability distributions to obtain an *estimated* cost per operation.

Amortized Analysis: Basics

Warning

Even if the amortized cost of one operation is $O(1)$, the worst-case cost of one particular operation may be substantially greater!

- Hence, studying amortized costs might not be good enough when a guaranteed low worst-case cost per operation is required. (E.g., for real-time or parallel systems.)
- We use dynamic arrays as a simple application to illustrate amortized analysis.
- Recall that inserting a new element at the end is the only costly operation; all other operations (are assumed to) run in $O(1)$ time in the worst case.
- Hence, we can focus on sequences of insertions.
- Three approaches to amortized analysis:
  - Aggregate analysis;
  - Accounting method;
  - Potential method.
- We apply the first two methods to the analysis of dynamic arrays.
- Note, though, that these three methods need not be equally suited for the analysis of some particular problem.

Amortized Analysis: Aggregate Method for Analyzing Dynamic Arrays

- Aggregate analysis determines an upper bound $U(n)$ on the total cost of a sequence of n operations.
- Then the amortized cost per operation is ${}^{U(n)}/_{n}$, i.e., all types of operations performed in the sequence have the same amortized cost.
- Suppose that the initial capacity of the array is 1, and that $\alpha := 2$.
- Then the cost c_i of the i-th insertion is

$$c_i = \begin{cases} i & \text{if } i-1 \text{ is a power of 2,} \\ 1 & \text{otherwise.} \end{cases}$$

- We get for the cost of n insertions

$$U(n) = \sum_{i=1}^{n} c_i = \left(\sum_{\substack{i=1 \\ (i-1) \text{ is no power of 2}}}^{n} 1 \right) + \left(\sum_{\substack{i=1 \\ (i-1) \text{ is power of 2}}}^{n} ((i-1)+1) \right)$$

$$= n + \sum_{i=0}^{\lfloor \log n \rfloor} 2^i = n + 2^{\lfloor \log n \rfloor + 1} - 1 \leq n + 2 \cdot 2^{\log n} = n + 2n = 3n.$$

- Hence, the amortized cost per (insertion) operation is ${}^{U(n)}/_{n} = \frac{3n}{n} \in O(1)$.

Amortized Analysis: Accounting Method

- One of the main shortcomings of aggregate analysis is that different types of operations are assigned the same amortized cost.
- As a natural improvement, one might want to assign different costs to different operations.
- The accounting method (aka banker's method) assigns charges to each type of operation.
- The amount charged for each type of operation is the amortized cost for that type.
- Some operations are overcharged while some other operations are undercharged.
- The balance is kept in a bank account:
  - Overcharged operations: If the charge is greater than the actual cost, then money can be saved and a *credit* accumulates in the bank account.
  - Undercharged operations: If the charge is less than the actual cost, then money is taken from the bank count to compensate the excess cost.

Amortized Analysis: Accounting Method

No debt!

Denote the (real) cost of the i-th operation by c_i and the amortized cost (i.e., charge) by $\hat{c}_i$. Then we require

$$\sum_{i=1}^{n} c_i \leq \sum_{i=1}^{n} \hat{c}_i$$

for every $n \in \mathbb{N}$ and every permissible sequence of n operations.

- If the charging scheme is not entirely trivial then one will have to resort to induction, loop invariants (or the like) in order to prove that the charging scheme of the accounting method works.

Amortized Analysis: Accounting Method for Analyzing Dynamic Arrays

- Recall that the cost c_i of the i-th insertion at the end of the dynamic array is

$$c_i = \begin{cases} i & \text{if } i-1 \text{ is a power of 2,} \\ 1 & \text{otherwise,} \end{cases}$$

  while all other operations have a cost of 1.
- We set the charge $\hat{c}_i$ for the i-th operation to 3 if it is an insertion, and to 1 otherwise.
- We claim that this charging scheme will result in a bank account that is always positive.
- Since all operations except insertions cost as much as we pay for, insertions are the only operations that we need to care about.

Amortized Analysis: Accounting Method

Charging scheme keeps positive account

The bank account is always positive after the insertion of the i-th element, for all $i \in \mathbb{N}$.

Proof :
I.B.: For $i := 1$ there is one element in the array and $\hat{c}_1 - c_1 = 2$ in the bank account. For $i := 2$ we have two elements in the array and $2 + 3 - 2 = 3$ in the bank account.
I.H.: The bank account is positive after the insertion of the j-th element, for some arbitrary but fixed $i \in \mathbb{N}$ with $i \geq 2$ and all $j \in \{1, 2, \ldots, i\}$.
I.S.: Since $\hat{c}_{i+1} - c_{i+1} = 2$, the bank account remains positive if the insertion of the $(i+1)$-st element does not require to resize the array.
So suppose that $(i+1) - 1 = 2^k$ for $k \in \mathbb{N}$. By the I.H. we know that the bank account was not negative when we doubled from a capacity of 2^{k-1} to 2^k. After doubling we inserted 2^{k-1} new elements into the table of capacity 2^k, saving $2 \cdot 2^{k-1} = 2^k$. This credit can be used to move all 2^k elements when doubling from 2^k to 2^{k+1}, and the bank account contains at least $3 - 1 = 2$ after the insertion of the element with number $i + 1 = 2^k + 1$. □

Amortized Analysis of Increments of a Binary Counter

- If we need to store a (possibly large) binary counter then it is natural to resort to an array and let the array element $A[i]$ store the i-th bit of the counter.
- The standard way of incrementing the counter is to toggle the lowest-order bit. If that bit switches to a 0 then we toggle the next higher-order bit, and so forth until the bit that we toggle switches to a 1 at which point we can stop.
- If we have n increment operations on a k-bit counter then the overall complexity is at most $O(k \cdot n)$. Note that, possibly, $k \gg n$. Can we do better?
- The result of the i-th increment is the number i (if we started at 0). Hence, after n increments at most $O(\log n)$ bits can have been toggled per increment, yielding a total of $O(n \log n)$ bits that need to be toggled.
- Is $O(n \log n)$ a tight bound? Can we do even better?

```
Increment(binaryArray A) {
   i = 1;
   while ((i < A.length) && (A[i] != 0)) {
      A[i] = 0;
      ++i;
   }
   if (i < A.length)   A[i] = 1;
}
```

Amortized Analysis of Increments of a Binary Counter

- *Aggregate method:* When does the i-th bit need to be toggled?
- $A[1]$ is toggled every time, $A[2]$ is toggled every other time, and $A[3]$ is toggled every fourth time.
- In general, bit $A[i]$ is toggled $\lfloor n/2^{i-1} \rfloor$ many times.
- Hence, for a sequence of n increments we get

$$\sum_{i=1}^{n} \left\lfloor \frac{n}{2^{i-1}} \right\rfloor = \sum_{i=0}^{n-1} \left\lfloor \frac{n}{2^{i}} \right\rfloor \le \sum_{i=0}^{n-1} \frac{n}{2^i} = n \sum_{i=0}^{n-1} \frac{1}{2^i} \le n \sum_{i=0}^{\infty} \frac{1}{2^i} = 2n$$

  as the total amortized cost.
- Thus, we get 2 as the amortized cost of one increment.

Practical Relevance of Worst-Case and Average-Case Analysis

Worst-case analysis:

- Worst-case analysis tends to be far too pessimistic for practical instances of a problem: A worst-case running time may be induced by pathological instances that do not resemble real-world instances.
- Famous example: Simplex method for solving linear optimization problems.

Average-case analysis:

- It gives the expected performance of a random input.
- Key problem: What is a good probability distribution for the input??
- Simply taking a uniform or Gaussian distribution tends to lead to incorrect results since it is based on the assertion that practical inputs have some specific properties with high probability.

Smoothed analysis:

- Introduced by Spielman and Teng in 2001.
- It models the expected performance of an algorithm under slight random perturbations of worst-case inputs.
- If the smoothed complexity is much lower than the average-case complexity then we know that the worst case is bound to occur only for few isolated problem instances.

Practical Relevance of Log-Terms

- Since $2^{20} = 1\,048\,576$ and $2^{30} = 1\,073\,741\,824$, in most applications the value of $\log n$ will hardly be significantly greater than 30 for practically relevant input sizes n.
- Hence, shaving off a multiplicative log-factor might constitute an important accomplishment when seen from a purely theoretical point of view, but its practical impact is likely to be much more questionable.
- In particular, multiplicative constants hidden in the O-terms may easily diminish the actual difference in speed between, say, an $O(n)$-algorithm and an $O(n \log n)$-algorithm.

Run-time experiments

Do not rely purely on experimental analysis to “detect” a log-factor: The difference between $\log(1024) = \log 2^{10}$ and $\log(1\,073\,741\,824) = \log 2^{30}$ is just a multiplicative factor of three!

Impact of Compile-Time Optimization

- Optimizing compilers try to minimize important characteristics of a program, such as its CPU-time consumption.
- Some problems related to code optimization are $\mathcal{NP}$-complete or even undecidable.
- Hence, several heuristics are employed that transform a program to a (hopefully) sementically equivalent program.
- E.g., an optimizing compiler will attempt to keep frequently used variables in registers rather than in main memory.
- Optimization may also involve the re-ordering of code or loop unrolling.
- C/C++: `gcc -O2`.

No speed-up guaranteed

In general, an optimized code will run faster. But optimization is not guaranteed to improve performance in all cases! It may even impede performance . . .

Impact of Compile-Time Optimization: Matrix Multiplication

Definition 66 (*Matrix multiplication*)

Let **A** be a matrix of size $m \times n$ and **B** be a matrix of size $n \times p$; that is, the number of columns of **A** equals the number of rows of **B**. Then $\mathbf{A} \cdot \mathbf{B}$ is the $m \times p$ matrix $\mathbf{C} = [c_{ij}]$ whose (i, j)-th element is defined by the formula

$$c_{ij} := \sum_{k=1}^{n} a_{ik} b_{kj} = a_{i1} b_{1j} + \cdots + a_{in} b_{nj}.$$

- Standard way to code matrix multiplication (for square matrices):

```
for (i = 0; i < n; i++) {
   for (j = 0; j < n; j++) {
      sum = 0;
      for (k = 0; k < n; k++)    sum += a[i][k] * b[k][j];
      c[i][j] = sum;
   }
}
```

Impact of Compile-Time Optimization: Matrix Multiplication

- Sample timings (in milliseconds) for the multiplication of two square matrices (with random integer elements).
- Platform: Intel^{TM} Core^{TM} i7-6700 CPU @3.40 GHz.

n	100	500	1000	2000	5000
`gcc -O0`	2.27	257.68	1943.27	10 224.13	216 154.34
`gcc -O2`	0.68	72.58	356.09	3606.34	85 682.03

- Note that $\frac{3606}{356} \approx 2.16^3$ and $\frac{85682}{3606} \approx 2.98^3$.

```
    for (i = 0; i < n; i++) {
       for (j = 0; j < n; j++) {
          sum = 0;
          for (k = 0; k < n; k++)    sum += a[i][k] * b[k][j];
          c[i][j] = sum;
       }
    }
```

Floating-Point Arithmetic and Compilers

- Be warned that x87 floating-points unit on x86 processors use 80bit registers and operators, while “double” variables are stored in 64bit memory cells.
- Hence, rounding to a lower precision is necessary whenever a floating-point variable is transferred from register to memory.
- Optimizing compilers analyze code and keep variables within the registers whenever this makes sense, without storing intermediate results in memory.
- As a consequence of this excess precision of the register variables, on my PC,

$$\sum_{i=1}^{1000000} 0.001 = 1000.0000000000009095 \qquad \text{with } \texttt{gcc -O2 -mfpmath=387},$$

$$\sum_{i=1}^{1000000} 0.001 = 999.9999999832650701 \qquad \text{with } \texttt{gcc -O0 -mfpmath=387}.$$

- Newer chips also support the SSE/SSE2 instruction sets, and the default option `-mfpmath=sse` avoids this particular problem for x86-64 compilers.

Warning

The result of fp-computations may depend on the compile-time options! Watch out for `-ffast-math` optimizations in GCC/Clang!

Dealing with Floating-Point Computations

- Theory tells us that we can approximate the first derivative f' of a function f at the point x_0 by evaluating $\frac{f(x_0+h)-f(x_0)}{h}$ for sufficiently small values of h ...
- Consider $f(x) := x^3$ and $x_0 := 10$:

$h := 10^0$:	$f'(10) \approx 331.0000000$	$h := 10^{-1}$:	$f'(10) \approx 303.0099999$
$h := 10^{-2}$:	$f'(10) \approx 300.3000999$	$h := 10^{-3}$:	$f'(10) \approx 300.0300009$
$h := 10^{-4}$:	$f'(10) \approx 300.0030000$	$h := 10^{-5}$:	$f'(10) \approx 300.0002999$
$h := 10^{-6}$:	$f'(10) \approx 300.0000298$	$h := 10^{-7}$:	$f'(10) \approx 300.0000003$
$h := 10^{-8}$:	$f'(10) \approx 300.0000219$	$h := 10^{-9}$:	$f'(10) \approx 300.0000106$
$h := 10^{-10}$:	$f'(10) \approx 300.0002379$	$h := 10^{-11}$:	$f'(10) \approx 299.9854586$
$h := 10^{-12}$:	$f'(10) \approx 300.1332515$	$h := 10^{-13}$:	$f'(10) \approx 298.9963832$
$h := 10^{-14}$:	$f'(10) \approx 318.3231456$	$h := 10^{-15}$:	$f'(10) \approx 568.4341886$
$h := 10^{-16}$:	$f'(10) \approx 0.000000000$	$h := 10^{-17}$:	$f'(10) \approx 0.000000000$

- The cancellation error increases as the step size, h, decreases. On the other hand, the truncation error decreases as h decreases.
- These two opposing effects result in a minimum error (and "best" step size h) that is high above the machine precision!

Dealing with Floating-Point Computations

- This gap between the theory of the reals and floating-point practice has important and severe consequences for the actual coding practice when implementing (geometric) algorithms that require floating-point arithmetic:
  1. The correctness proof of the mathematical algorithm does not extend to the program, and the program can fail on seemingly appropriate input data.
  2. Local consistency need not imply global consistency.

Numerical analysis . . .

. . . and adequate coding are a must when implementing algorithms that deal with real numbers. Otherwise, the implementation of an algorithm may turn out to be absolutely useless in practice, even if the algorithm (and even its implementation) would come with a rigorous mathematical proof of correctness!

Impact of Cache Misses

- Today's computers perform arithmetic and logical operations on data stored in registers.
- In addition to main memory, data can also be stored in a Level 1 cache or a Level 2 cache. (Multi-core machines tend to have also L3 caches.)
- In a nutshell:
  - A cache is a fast but expensive memory which holds the values of standard memory locations.
  - If the CPU requests the value of a memory location and if that value is available in some level of the cache, then the value is fetched from the cache, at a cost of a few cycles: *cache hit*.
  - Otherwise, a block of consecutive memory locations is accessed and brought into the cache: *cache miss*.
  - A cache miss is much costlier than a cache hit!
- Since the gap between CPU speed and memory speed gets wider and wider, good cache management and programs that exhibit good *locality* become increasingly more important.

Impact of Cache Misses: Matrix Multiplication Revisited

- C/C++: Elements within the same row of a matrix are stored in consecutive memory locations, while elements in the same column may be far apart in main memory.
- The standard implementation of matrix multiplication causes the elements of **A** and **C** to be accessed row-wise, while the elements of **B** are accessed by column.
- This will result in a lot of cache misses if **B** is too large to fit into the (L2) cache.

```
for (i = 0; i < n; i++) {
   for (j = 0; j < n; j++) {
      sum = 0;
      for (k = 0; k < n; k++)    sum += a[i][k] * b[k][j];
      c[i][j] = sum;
   }
}
```

Impact of Cache Misses: Matrix Multiplication Revisited

- Rewriting of the standard multiplication algorithm (“ijk-order”).
- Re-ordering of the inner loops will cause the matrices **B** and **C** to be accessed row-wise within the inner-most loop, while the indices i, k of the (i, k)-th element of **A** remain constant: “ikj-order”.

```
for (i = 0; i < n; i++) {
   for (j = 0; j < n; j++)  c[i][j] = 0;
}
for (i = 0; i < n; i++) {
   for (k = 0; k < n; k++) {
      for (j = 0; j < n; j++) {
         c[i][j] += a[i][k] * b[k][j];
      }
   }
}
```

Impact of Cache Misses: Matrix Multiplication Revisited

- Platform: Intel^{TM} Core^{TM} i7-6700 CPU @3.40 GHz.
- Caches: 256KiB L1, 1MiB L2, 8MiB L3.
- CPU-time consumption of ikj-order matrix multiplication divided by the CPU-time consumption of the standard ijk-order matrix multiplication.

	N	100	500	1000	2000	5000
`gcc -O0`	$^{ikj}/_{ijk}$	1.596	1.112	1.090	0.911	0.678
`gcc -O2`	$^{ikj}/_{ijk}$	0.882	0.805	0.719	0.602	0.389

Cache misses

Avoiding cache misses may result in a substantially faster program!

Theory and Practice

- Algorithms (and corresponding codes) employed by industry need not be the algorithms taught in an academic course.
- That is, there is a gap between theory and practice . . .

Benjamin Brewster ("The Yale Literary Magazine" 1882)

In theory, there is no difference between theory and practice. In practice, there is.

Marie von Ebner-Eschenbach (1893)

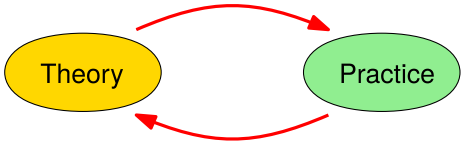
Theorie und Praxis sind eins wie Seele und Leib, und wie Seele und Leib liegen sie großenteils miteinander in Streit.

Jan L.A. van de Snepscheut

The difference between theory and practice is larger in practice than the difference between theory and practice in theory.

Theory Into Practice

What we'd need . . .



Ayn Rand (Russian-born American writer and philosopher)

Those who say that theory and practice are two unrelated realms are fools in one and scoundrels in the other.

Folklore ☻

Theory is when you know everything but nothing works. Practice is when everything works but no one knows why. However, we combine theory and practice: Nothing works and no one knows why.

Algorithm Engineering

- Recent observation of one of my MSc. students: A smarter reallocation of a vector reduced the runtime from 6000 µs to 7000 µs down to 1 µs to 4 µs.
- The bottom line is that algorithms may need some tweaking to make them fit practical needs and to make them run fast for practical problems.

Algorithm engineering . . .

. . . is a cycle of design, analysis, implementation, profiling and experimental evaluation that attempts to produce more efficient algorithms for practical instances of problems.

Algorithm engineering . . .

. . . should be standard when designing and implementing an algorithm! Decent algorithm engineering may pay off more significantly than attempting to implement a highly complicated algorithm just because its theoretical analysis predicts a better running time.

Algorithmic Paradigms

Incremental Construction
Greedy
Divide and Conquer
Dynamic Programming
Randomization

Incremental Construction

Incremental construction

A result $R(\{x_1, x_2, \ldots, x_n\})$ that depends on n input items $x_1, x_2, \ldots, x_n$ is computed by dealing with one item at a time: For $2 \leq i \leq n$, we obtain $R(\{x_1, x_2, \ldots, x_i\})$ from $R(\{x_1, x_2, \ldots, x_{i-1}\})$ by "inserting" the i-th item x_i into $R(\{x_1, x_2, \ldots, x_{i-1}\})$.

Important invariant of incremental construction

$R(\{x_1, x_2, \ldots, x_i\})$ exhibits all the desired properties of the final result $R(\{x_1, x_2, \ldots, x_n\})$ restricted to $\{x_1, x_2, \ldots, x_i\}$ as input items: If we would stop incremental construction after having inserted x_i then we would have the correct solution $R(\{x_1, x_2, \ldots, x_i\})$ for $\{x_1, x_2, \ldots, x_i\}$.

- Once this invariant has been established the overall correctness of an incremental algorithm is a simple consequence.
- The total complexity is given as a sum of the complexities of the individual "insertions".
- Incremental algorithms are particularly well suited for dealing with "online problems", for which data items arrive one after the other. (Of course, only if you can afford the time taken by the subsequent insertions.)

Incremental Construction: Insertion Sort

- Insertion sort is a classical incremental algorithm: We insert the i-th item (of n items) into the sorted list of the first $i-1$ items, thereby transforming it into a sorted list of the first i items.

```
InsertionSort(array A[], int low, int high)
{
   for (i = low+1;  i <= high;  ++i) {
      x = A[i];
      j = i;
      while ((j > 1) && (A[j-1] > x)) {
         A[j] = A[j - 1];
         --j;
      }
      A[j] = x;
   }
}
```

- $O(n)$ for pre-sorted input, $O(n^2)$ worst case; efficient for small arrays.
- Adaptive (i.e., efficient for substantially sorted input), stable, in-place and online.
- Library sort maintains small chunks of unused spaces throughout the array and runs in $O(n \log n)$ time with high probability [Farach-Colton&Mosteiro (2006)].

Incremental Construction: Convex Hull

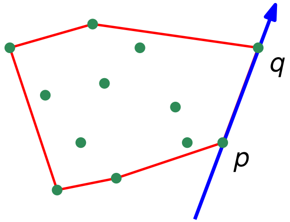
Problem: ConvexHull

Input: A set S of n points in the Euclidean plane $\mathbb{R}^2$.

Output: The convex hull $CH(S)$, i.e., the smallest convex super set of S.

Lemma 67

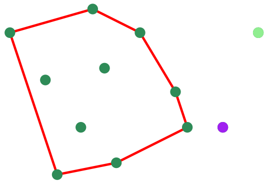
1. The convex hull of a set S of points in $\mathbb{R}^2$ is a convex polygon.
2. Two distinct points $p, q \in S$ define an edge of $CH(S)$ if and only if all points of $S \setminus \{p, q\}$ lie on one side of the line through p, q.

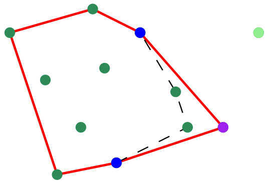


Incremental Construction: Convex Hull

1. Sort the points according to their x-coordinates, and re-number accordingly: $S := \{p_1, p_2, \ldots, p_n\}$. (Suppose that all x-coordinates are distinct.)
2. Compute $CH(\{p_1, p_2, p_3\})$.
3. Suppose that $CH(\{p_1, p_2, \ldots, p_{i-1}\})$ is known. We insert p_i.
   - **3.a** Compute the supporting lines of $CH(\{p_1, p_2, \ldots, p_{i-1}\})$ and p_i.
   - **3.b** Split $CH(\{p_1, p_2, \ldots, p_{i-1}\})$ into two parts at the two vertices of $CH(\{p_1, p_2, \ldots, p_{i-1}\})$ where the supporting lines touch.
   - **3.c** Discard that part of $CH(\{p_1, p_2, \ldots, p_{i-1}\})$ which faces p_i.

- What is the complexity of this incremental construction scheme?
- Recall Corollary 63: The worst-case complexity of ConvexHull for n points has an $\Omega(n \log n)$ lower bound in the ACT model.





Incremental Construction: Convex Hull

Naïve complexity analysis:

- The initial sorting takes $O(n \log n)$ time.
- The construction of $CH(\{p_1, p_2, p_3\})$ takes $O(1)$ time.
- Inserting p_i into $CH(\{p_1, p_2, \ldots, p_{i-1}\})$ will result in discarding one or more vertices of $CH(\{p_1, p_2, \ldots, p_{i-1}\})$ and, thus, takes $O(i)$ time.
- Hence we get

$$O(n \log n) + O(1) + O(4 + 5 + \ldots + n) = O(n^2)$$

as total time complexity.

Amortized complexity analysis:

- Let m_i denote the number of vertices that are discarded from $CH(\{p_1, p_2, \ldots, p_{i-1}\})$ when p_i is inserted.
- Then the insertion of p_i takes $O(m_i + 1)$ time.
- Observation: $m_4 + m_5 + \ldots m_n < n$.
- Hence, the insertion of p_i runs in amortized time $O(1)$, and the total complexity of the incremental construction algorithm is $O(n \log n)$.

Theorem 68

The convex hull of n points in the plane can be computed in worst-case optimal time $O(n \log n)$ by means of incremental construction.

Greedy Paradigm

- A *greedy algorithm* attempts to solve an optimization problem by repeatedly making the locally best choice in a hope to arrive at the global optimum.
- A greedy algorithm may but need not end up in the optimum. E.g., greedy solution for ETSP-COMP or cashier's algorithm for coin changing.
- If a greedy algorithm is applicable to a problem then the problem tends to exhibit the following two properties:

  Optimal substructure: The optimum solution to a problem consists of optimum solutions to its sub-problems.

  Greedy choice property: Choices may depend on prior choices, but must not depend on future choices; no choice is reconsidered.
- If a greedy algorithm does indeed produce the optimum solution then it likely is the algorithm of choice since it tends to be faster than other algorithms (e.g., based on dynamic programming).
- Success stories: Kruskal's algorithm and Prim's algorithm for computing minimum spanning trees.

Greedy Paradigm: Selection Sort

- Selection sort is a classical greedy algorithm: We sort the array by repeatedly searching the k-smallest item and moving it forward to make it the k-th item of the array.

```
SelectionSort(array A[], int low, int high)
{
   for (i = low;  i < high;  ++i) {
      int j_min = i;
      for (j = i+1;  j <= high;  ++j) {
         if (A[j] < A[j_min])  j_min = j;
      }
      if (j_min != i)  Swap(A[i], A[j_min]);
   }
}
```

- Selection sort runs in $O(n^2)$ time in both the average and the worst case. Its running time tends to be inferior to that of insertion sort.
- However, it requires only $O(n)$ write operations of array elements while insertion sort may consume $O(n^2)$ write operations.

Greedy Paradigm: Huffman Coding

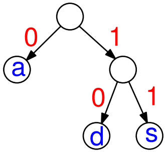
- Standard encoding schemes of symbols use a fixed number of bits to encode each symbol.
- E.g., ASCII encoding uses seven bits to encode the lowest 128 Unicode characters, from U+0000 to U+007F.
- Decoding an ASCII string is easy: Scan it in chunks of seven bits and look up the corresponding symbol.
- Encodings like ASCII do not take the frequency of occurrence of the indvidual symbols into account.
- One can achieve a (lossless) compression by encoding symbols that occur
  - more frequently (such as the letters “e” and “a”) with shorter bit strings;
  - less frequently (such as the letter “q”) with longer bit strings.
- Obvious problem for variable-length encodings: If one would assign, say, `1` to “a” and `11` to “q” then an encoding string that starts with `11` cannot be decoded unambiguously.

Greedy Paradigm: Huffman Coding

Definition 69 (*Prefix code, Dt.: Präfixcode, präfixfreier Code*)

Consider a set Ω of symbols. A *prefix code* for Ω is a function c that maps every $x \in \Omega$ to a binary string, i.e., to a sequence of 0s and 1s, such that $c(x)$ is not a prefix of $c(y)$ for all $x, y \in \Omega$ with $x \neq y$.

$$\Omega := \{a, d, s\}$$
$$c(a) := 0$$
$$c(d) := 10$$
$$c(s) := 11$$



- Hence, 001011 corresponds to “aads”.

- A prefix code is also said to have the *prefix property*.
- Real-world examples of prefix codes:
  - Country dial-in codes used by member countries of the International Telecommunication Union.
  - Machine language instructions of most computer architectures.
  - Country and publisher encoding within ISBNs.

Greedy Paradigm: Huffman Coding

Lemma 70

Let $\mathcal{T}$ be the binary tree that represents the encoding function c. If c is a prefix code for Ω then only the leaves of $\mathcal{T}$ represent symbols of Ω.

Definition 71 (*Average number of bits per symbol*)

Consider a set Ω of symbols and a frequency function $f\colon \Omega \to \mathbb{R}^+$. The *average number of bits per symbol* of a prefix code c is given by

$$ANBS(\Omega, c, f) := \sum_{\omega \in \Omega} f(\omega) \cdot |c(\omega)|,$$

where $|c(\omega)|$ denotes the number of bits used by c to encode ω.

$$c(a) := 0 \qquad f(a) := 0.5$$
$$c(d) := 10 \qquad f(d) := 0.3$$
$$c(s) := 11 \qquad f(s) := 0.2$$

- Then, for $\Omega := \{a, d, s\}$, $ANBS(\Omega, c, f) = 0.5 \cdot 1 + 0.3 \cdot 2 + 0.2 \cdot 2 = 1.5$.

Definition 72 (*Optimum prefix code*)

A prefix code c^* for Ω is *optimum* if it minimizes $ANBS(\Omega, c, f)$ for a given frequency f.

Greedy Paradigm: Huffman Coding

- We call a binary tree $\mathcal{T}$ *full* if every non-leaf node of $\mathcal{T}$ has two children.

Lemma 73

If a prefix code c^* is optimum then the binary tree that represents c^* is a full tree.

Lemma 74

The lowest-frequency symbol of Ω appears at the lowest level of the tree that represents an optimum prefix code c^*.

Huffman's greedy template (1952)

1. Create two leaves for the two lowest-frequency symbols $s_1, s_2 \in \Omega$.
2. Recursively build the encoding tree for $(\Omega \cup \{s_{12}\}) \setminus \{s_1, s_2\}$, with $f(s_{12}) := f(s_1) + f(s_2)$, where s_{12} is a new symbol that does not occur in Ω.

Theorem 75

Huffman's greedy algorithm computes an optimum prefix code c^* for Ω relative to a given frequency f of the symbols of Ω.

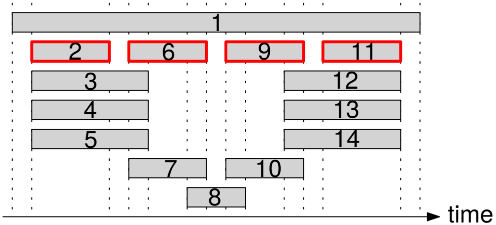
Greedy Paradigm: Job Scheduling

Problem: JOBSCHEDULING

Input: A set J of n jobs, where job i starts at time s_i and finishes at time f_i. Two jobs i and j are *compatible* if they do not overlap time-wise, i.e., if either $f_i \leq s_j$ or $f_j \leq s_i$.

Output: A maximum subset J' of J such that the jobs of J' are mutually compatible.

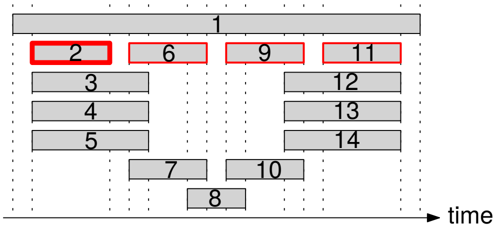
- Can we arrange the jobs in some "natural order", and pick jobs successively provided that a new job is compatible with the previously picked jobs?



Greedy Paradigm: Job Scheduling

- Can we consider the jobs in some “natural order”?

  Fewest conflicts: Pick jobs according to smallest number of incompatible jobs.
  Shortest job duration: Pick jobs according to ascending order of $f_i - s_i$.
  Earliest start time: Pick jobs according to ascending order of s_i.
  Earliest finish time: Pick jobs according to ascending order of f_i.



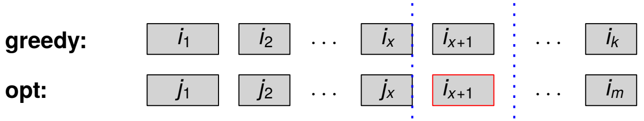
Greedy Paradigm: Job Scheduling

Lemma 76

Picking jobs according to earliest finish time allows to compute an optimum solution to JOBSCHEDULING in $O(n \log n)$ time for n jobs.

Proof :

- It is obvious that sorting the n jobs in ascending order of f_i allows to generate a solution in $O(n \log n)$ time. W.l.o.g., $f_i \neq f_j$ if $i \neq j$.
- Suppose that an optimum solution has m jobs while a greedy approach picks $k < m$ jobs $i_1, i_2, \ldots, i_k$.
- Let x be the largest-possible number such that $i_1 = j_1, i_2 = j_2, \ldots, i_x = j_x$, over all optimum solutions $j_1, j_2, \ldots, j_m$. We have $x < m$.
- A compatible job i_{x+1} exists that finishes earlier than job j_{x+1}, i.e., $f_{i_{x+1}} < f_{j_{x+1}}$.
- Replacing job j_{x+1} by job i_{x+1} in the optimum solution maintains optimality, but violates maximality of x.



□

Greedy Paradigm: Processor Scheduling

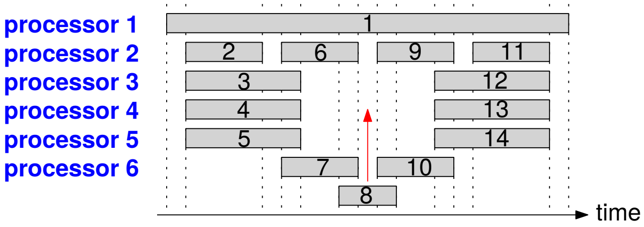
Caveat

Seemingly similar problems may require different greedy strategies!

Problem: ProcessorScheduling

Input: A set J of n jobs, where job i starts at time s_i and finishes at time f_i. Two jobs i and j are *compatible* if they do not overlap time-wise.

Output: An assignment of all jobs to a minimum number of processors such that no two incompatible jobs run on the same processor.



Lemma 77

Assigning jobs according to earliest start time allows to compute an optimum solution to ProcessorScheduling in $O(n \log n)$ time.

Divide&Conquer: Basics

- Gaius Julius Caesar (100–44 BCE): “Divide et impera”. However, this maxim seems to go back to Philip II of Macedon (382–336 BCE).

Basic principle

- Let S denote the input set and let n denote the size of S.
- If $n = 1$ then (process S and) return to calling level.
- Otherwise:
  - Partition S into subproblems of size at most $f(n)$.
  - Solve each of the $n/f(n)$ subproblems recursively.
  - Combine solutions of these subproblems and return to calling level.

- The function f has to satisfy the contraction condition $f(n) < n$ for $n > 1$.
- If partitioning S into subproblems and combining the solutions of these subproblems runs in linear time then we get the following recurrence relation for the time complexity T for a suitable $a \in \mathbb{N}$:

$$T(n) = \frac{n}{f(n)} \cdot T(f(n)) + a \cdot n$$

Divide&Conquer: Basics

- Standard analysis yields

$$T(n) \leq a \cdot n \cdot f^*(n)$$

for $f^* : \mathbb{N}_0 \to \mathbb{R}_0^+$ with

$$f^*(n) := \begin{cases} 0 & \text{if } n \leq 1, \\ 1 + f^*(f(n)) & \text{if } n > 1. \end{cases}$$

- That is,

$$f^*(n) = \min\{k \in \mathbb{N}_0 : \underbrace{f(f(\ldots f(n)\ldots))}_{k \text{ times}} \leq 1\}.$$

- Sample results for f^* and a constant $c \in \mathbb{N}$ with $c \geq 2$:

$f(n)$	$n-1$	$n-c$	$^n/_c$	$\sqrt{n}$	$\log n$
$f^*(n)$	$n-1$	$^n/_c$	$\log_c n$	$\log \log n$	$\log^* n$

Divide&Conquer: Merge Sort

```
MergeSort(array A[], int low, int high)
{
   int i;          /* counter */
   int middle;     /* index of middle element */
   if (low < high) {
      middle = (low+high) / 2;
      MergeSort(A, low, middle);
      MergeSort(A, middle+1, high);
      Merge(A, low, middle, high);
   }
}
```

- Always try to divide the job evenly!
- Does it matter if you cannot guarantee to split exactly in half? No! It is good enough to ensure that the size of every sub-problem is at most some constant fraction of the original problem size. (At least as far as the asymptotic complexity is concerned.)

Divide&Conquer: Fast Matrix Multiplication

- Recall: If **A**, **B** are two square matrices of size $n \times n$, then $\mathbf{A} \cdot \mathbf{B}$ is the $n \times n$ matrix $\mathbf{C} = [c_{ij}]$ whose (i, j)-th element c_{ij} is defined by the formula

$$c_{ij} := \sum_{k=1}^{n} a_{ik} b_{kj} = a_{i1} b_{1j} + \cdots + a_{in} b_{nj}.$$

- Standard multiplication of two $n \times n$ matrices results in $\Theta(n^3)$ many arithmetic operations.

Theorem 78 (*Strassen (1969)*)

Seven multiplications of scalars suffice to compute the multiplication of two 2×2 matrices. In general, $O(n^{\log_2 7}) \approx O(n^{2.807\ldots})$ arithmetic operations suffice for $n \times n$ matrices.

- Strassen's algorithm is more complex and numerically less stable than the standard naïve algorithm. But it is considerably more efficient for large n, i.e., roughly when $n > 100$, and it is very useful for large matrices over finite fields.
- It does not assume multiplication to be commutative and, thus, works over arbitrary rings.

Divide&Conquer: Fast Matrix Multiplication

Proof of Thm. 78 for $n = 2$: For $\mathbf{A}, \mathbf{B} \in M_{2\times 2}$, we compute

$$\mathbf{C} = \mathbf{A} \cdot \mathbf{B} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} \cdot \begin{pmatrix} b_{11} & b_{12} \\ b_{21} & b_{22} \end{pmatrix}$$

via

$$\begin{aligned}
p_1 &:= (a_{12} - a_{22})(b_{21} + b_{22}) \\
p_2 &:= (a_{11} + a_{22})(b_{11} + b_{22}) \\
p_3 &:= (a_{11} - a_{21})(b_{11} + b_{12}) \\
p_4 &:= (a_{11} + a_{12})b_{22} \\
p_5 &:= a_{11}(b_{12} - b_{22}) \\
p_6 &:= a_{22}(b_{21} - b_{11}) \\
p_7 &:= (a_{21} + a_{22})b_{11}
\end{aligned}$$

and set

$$\begin{aligned}
c_{11} &:= a_{11}b_{11} + a_{12}b_{21} &&= p_1 + p_2 - p_4 + p_6 \\
c_{12} &:= a_{11}b_{12} + a_{12}b_{22} &&= p_4 + p_5 \\
c_{21} &:= a_{21}b_{11} + a_{22}b_{21} &&= p_6 + p_7 \\
c_{22} &:= a_{21}b_{12} + a_{22}b_{22} &&= p_2 - p_3 + p_5 - p_7 .
\end{aligned}$$

Obviously, this approach results in 7 multiplications and 18 additions/subtractions. □

Divide&Conquer: Fast Matrix Multiplication

Proof of Thm. 78 for $n = 2m$: For $\mathbf{A}, \mathbf{B} \in M_{2m\times 2m}$, we compute $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}$ by resorting to manipulating block matrices of size $m \times m$:

$$\begin{pmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{pmatrix} \cdot \begin{pmatrix} b_{11} & \cdots & b_{1n} \\ \vdots & \ddots & \vdots \\ b_{n1} & \cdots & b_{nn} \end{pmatrix} = \begin{pmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{pmatrix} \cdot \begin{pmatrix} \mathbf{B}_{11} & \mathbf{B}_{12} \\ \mathbf{B}_{21} & \mathbf{B}_{22} \end{pmatrix},$$

where $\mathbf{A}_{11}, \mathbf{A}_{12}, \mathbf{A}_{21}, \mathbf{A}_{22}, \mathbf{B}_{11}, \mathbf{B}_{12}, \mathbf{B}_{21}, \mathbf{B}_{22} \in M_{m\times m}$ with

$$\mathbf{A}_{11} = \begin{pmatrix} a_{11} & \cdots & a_{1m} \\ \vdots & \ddots & \vdots \\ a_{m1} & \cdots & a_{mm} \end{pmatrix}, \quad \mathbf{A}_{12} = \begin{pmatrix} a_{1,m+1} & \cdots & a_{1,2m} \\ \vdots & \ddots & \vdots \\ a_{m,m+1} & \cdots & a_{m,2m} \end{pmatrix},$$

$$\mathbf{A}_{21} = \begin{pmatrix} a_{m+1,1} & \cdots & a_{m+1,m} \\ \vdots & \ddots & \vdots \\ a_{2m,1} & \cdots & a_{2m,m} \end{pmatrix}, \quad \mathbf{A}_{22} = \begin{pmatrix} a_{m+1,m+1} & \cdots & a_{m+1,2m} \\ \vdots & \ddots & \vdots \\ a_{2m,m+1} & \cdots & a_{2m,2m} \end{pmatrix}.$$

Analogously for $\mathbf{B}_{11}, \mathbf{B}_{12}, \mathbf{B}_{21}, \mathbf{B}_{22}$. Then the approach used for multiplying 2×2 matrices can be applied, with a_{ij} and b_{ij} being replaced by $\mathbf{A}_{ij}$ and $\mathbf{B}_{ij}$, for $1 \le i, j \le 2$. That is, we have matrices rather than scalars as operands for addition and multiplication.

Divide&Conquer: Fast Matrix Multiplication

Proof of Thm. 78 for $n = 2m$ (cont'd) : Hence, we can compute $\mathbf{C} = \mathbf{A} \cdot \mathbf{B}$ by using

- 7 multiplications of $m \times m$ matrices,
- 18 additions/subtractions of $m \times m$ matrices.

Obviously, one addition of two $m \times m$ matrices takes $O(m^2)$ time, i.e., $O(n^2)$ time.

Let $T(n)$ denote the number of (arithmetic) operations consumed by Strassen's algorithm for multiplying two $n \times n$ matrices. We get the following recurrence relation for T:

$$T(n) = 7 \cdot T\left(\frac{n}{2}\right) + O(n^2).$$

The Master Theorem 32 yields

$$T \in \Theta(n^{\log_2 7}) \approx O(n^{2.807\ldots}). \qquad \square$$

Divide&Conquer: Fast Matrix Multiplication

- Strassen's algorithm is not the fastest algorithm for multiplying matrices.

Lemma 79 (*Coppersmith&Winograd (1990)*)

$O(n^{2.37547\dots})$ arithmetic operations suffice for multiplying two $n \times n$ matrices.

Lemma 80 (*Stothers (2010, 2013)*)

$O(n^{2.37369\dots})$ arithmetic operations suffice for multiplying two $n \times n$ matrices.

Lemma 81 (*Williams (2011, 2012), Le Gall (2014), Alman&Williams (2021)*)

$O(n^{2.37285\dots})$ arithmetic operations suffice for multiplying two $n \times n$ matrices.

- Open problem: What is the true lower bound?
- The Coppersmith-Winograd algorithm and the more recent improvements are used frequently as building blocks in other algorithms to prove complexity bounds. E.g., the best algorithm for computing the diameter of a graph runs in $O(n^\omega \log n)$ time, where ω is the so-called *exponent of matrix multiplication*.
- Besides Strassen's algorithm, these algorithms are of no practical value, though, since the cross-over point for where they would improve on the naïve cubic-time algorithm is enormous.

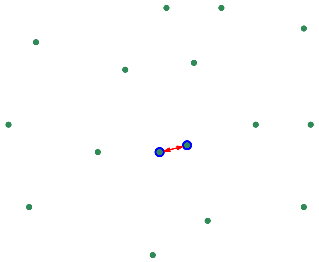
Divide&Conquer: Closest Pair

Problem: ClosestPair

Input: A set S of n points in the Euclidean plane.

Output: Those two points of S whose mutual distance is minimum among all pairs of points of S.

- Corollary 64: The worst-case complexity of ClosestPair for n points has an $\Omega(n \log n)$ lower bound in the ACT model of computation.
- Easy to solve in $O(n \log n)$ time if all points lie on the x-axis (or on a line).



Divide&Conquer: Closest Pair

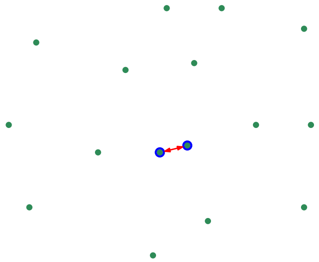
Problem: ClosestPair

Input: A set S of n points in the Euclidean plane.

Output: Those two points of S whose mutual distance is minimum among all pairs of points of S.

Lemma 82

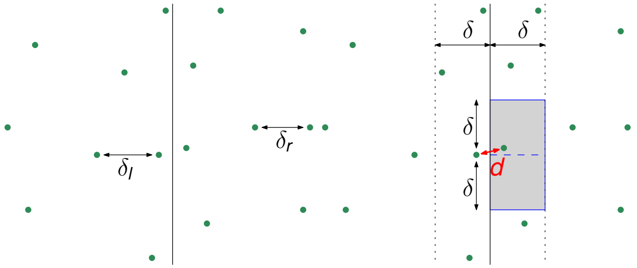
ClosestPair for n points can be solved in worst-case optimal time $O(n \log n)$.



Divide&Conquer: Closest Pair

Proof of Lemma 82 :

- Sort the points according to x-coordinates, and split at median x-coordinate into a left sub-set and a right sub-set.
- Recursively find the minimum distance in the left sub-set and in the right sub-set. Return the points sorted according to y-coordinates.
- Consider a strip of width 2δ, where $\delta := \min\{\delta_l, \delta_r\}$.
- Slide a window of height 2δ upwards within this strip and compute distances between those points of the left and the right sub-set which lie within this window.
- Merge the y-sorted points of the left and right sub-set.



Divide&Conquer: Closest Pair

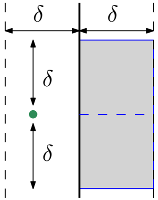
Proof of Lemma 82 (cont'd) : Time complexity:

- Sorting according to x-coordinates takes $O(n \log n)$ time.
- Splitting n vertices at median x-coordinate takes $O(n)$ time.
- The distance computations take $O(1)$ time for each position of the sliding window.
- Thus, all distance computations carried out during the conquer step run in $O(n)$ time.
- Merging the y-sorted points of the left and right sub-set takes $O(n)$ time.
- Hence, for the time complexity $T(n)$ we get

$$T(n) = 2T\left(\frac{n}{2}\right) + O(n), \quad \text{resulting in } T \in O(n \log n),$$

and, thus, an overall $O(n \log n)$ time bound. □

- Question: How many points of the right sub-set can lie within the sliding window?
- Answer: Only a constant number! (Eight is easy to argue, but one can prove six.)



Dynamic Programming

- In a nutshell, dynamic programming (DP) is a technique for efficiently implementing a recursive algorithm by storing results for sub-problems.
- It may be applicable if the naïve recursive algorithm would solve the same sub-problems over and over again. In that case, storing the solution for every sub-problem in a table to look up instead of re-compute may lead to a more efficient algorithm.
- The word "programming" in the term DP does not refer to classical programming at all. It was coined by Bellman in 1957.
- According to Rust [2006],

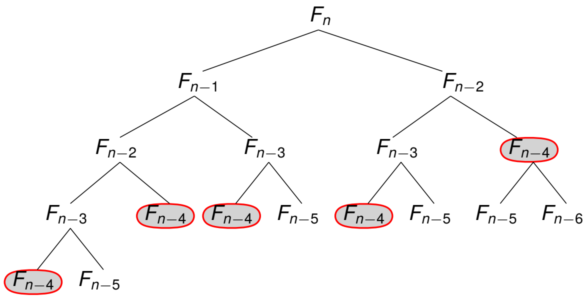
  Bellman explained that he invented the name "dynamic programming" to hide the fact that he was doing mathematical research at RAND under a Secretary of Defense who 'had a pathological fear and hatred of the term "research".' He settled on the term "dynamic programming" because it would be difficult to give a 'pejorative meaning' and because 'It was something not even a Congressman could object to.'

Dynamic Programming: Fibonacci Numbers

- Recall that the Fibonacci numbers are defined as follows:

$$F_n := \begin{cases} n & \text{if } n \leq 1, \\ F_{n-1} + F_{n-2} & \text{if } n \geq 2. \end{cases}$$

- Since the Fibonacci numbers are defined recursively, a recursive computation scheme seems natural ...
- Note that this requires Fibonacci numbers to be computed over and over again.
- E.g., F_{n-4} is computed five times, each time from scratch.
- What is the complexity of this approach?



Dynamic Programming: Fibonacci Numbers

- If we ignore the cost of adding two (possibly large) integers then we get

  $$C(n) := C(n-1) + C(n-2)$$

  as the cost $C(n)$ for computing the n-th Fibonacci number.
- This is the same recurrence as for the Fibonacci numbers!
- The theory of Fibonacci numbers (Lem. 5) tells us that

  $$F_n = \frac{1}{\sqrt{5}} \cdot \left(\frac{1+\sqrt{5}}{2}\right)^n - \frac{1}{\sqrt{5}} \cdot \left(\frac{1-\sqrt{5}}{2}\right)^n .$$

- Hence, we pay an exponential price for computing F_n recursively:

  $$C \in O(\phi^n), \quad \text{with the golden ratio } \phi := \frac{1+\sqrt{5}}{2}.$$

- The closed-form solution for F_n could be used to compute F_n using only $\Theta(\log n)$ many multiplications.
- But this would require us to deal with irrational numbers!

Dynamic Programming: Fibonacci Numbers

- A memoized DP approch allows to compute the n-th Fibonacci number in $O(n)$ steps (if we ignore the time needed to add large integers), using $O(n)$ memory.
- A simple bottom-up DP approach based on tabulation suffices to compute the n-th Fibonacci number also in $O(n)$ steps but with $O(1)$ memory.
- Note that it suffices to remember only the two numbers computed most recently.

```
int Fibonacci(int number) /* greater zero */
{
    int n1 = 0;
    int n2 = 1;
    int temp, i;
    for (i = 1;  i < number;  ++i) {
        temp = n1 + n2;
        n1 = n2;
        n2 = temp;
    }
    return n2;
}
```

Dynamic Programming: Traveling Salesman Problem

Problem: TRAVELINGSALESMANPROBLEM (TSP), DT.: RUNDREISEPROBLEM

Input: A weighted and undirected graph $\mathcal{G} := (V, E)$, and a number $c \in \mathbb{R}^+$.

Decide: Does $\mathcal{G}$ contain a Hamiltonian cycle whose total cost is less than c?

Naïve approach:

- Fix one node as start-/end-node and evaluate the costs of all $(n-1)!$ possible cycles.
- This approach takes $O(n!)$ time.

- TSP is an $\mathcal{NP}$-complete problem. (See later on.) Hence, there is little hope to devise an exact solution that runs in polynomial time.

Theorem 83 (*Bellman (1962), Held&Karp (1962)*)

Dynamic programmming allows to solve TSP for a weighted graph with n nodes in $O(n^2 \cdot 2^n)$ time, within $O(n \cdot 2^n)$ space.

Dynamic Programming: Traveling Salesman Problem

Proof of Theorem 83 :

- We number the nodes $1, 2, \ldots, n-1, n$, denote the weight of the edge between i and j by w_{ij}, and designate node 1 as start-/end-node of the TSP cycle.
- Of course, $w_{ij} = w_{ji}$, and $w_{ij} := \infty$ if $\{i, j\} \notin E$.
- For a subset of nodes $S \subseteq \{2, 3, \ldots, n\}$, and $j \in S$, let $C(S, j)$ be the length of the cheapest path starting at 1 and ending at j that visits each node in S exactly once.
- If $S = \{j\}$ then $C(S, j) := d_{1j}$.
- Now assume that $|S| \geq 2$ and let $i \in S$ be the second-to-last node on a path from 1 to j within S. Then the minimum cost of that path is given by the cost of the cheapest path from 1 to i within $S \setminus \{j\}$ plus w_{ij}.
- Hence, $C(S, j)$ is obtained by minimizing over $|S| - 1$ paths within S:

$$C(S, j) = \min_{i \in (S \setminus \{j\})} \Big(C(S \setminus \{j\}, i) + w_{ij} \Big).$$

- Then the final cost of a TSP cycle is given by

$$\min_{j \in \{2,3,\ldots,n\}} C(\{2, \ldots, n\}, j) + d_{j1}.$$

- Of course, the subsets S of $\{2, 3, \ldots, n\}$ are processed in order of increasing cardinality.

Dynamic Programming: Traveling Salesman Problem

Proof of Theorem 83 (cont'd) :

Space complexity:

- There are 2^{n-1} subsets S of $\{2, 3, \ldots, n\}$.
- For every subset S we have to know (and store) $C(S, j)$ for all $j \in S$.
- Hence, if we assume that n is sufficiently small such that S can be encoded by a bitmask of a constant number of machine words (rather than by $|S|$-tuples), then the space complexity is $O(n \cdot 2^n)$.

Time complexity:

- $C(S, j)$ is computed in linear time from the items computed previously.
- Hence, the time complexity is $O(n^2 \cdot 2^n)$.

□

- The actual TSP cycle can be obtained by storing with every $C(S, j)$ the index of the second-to-last node i on the cheapest path from 1 to j.

Dynamic Programming

Dynamic programming . . .

. . . may result in an efficient (sub-exponential) algorithm if the following conditions hold:

- A solution can be computed by combining solutions of sub-problems;
- A solution of every sub-problem can be computed by combining solutions of sub-subproblems; etc.
- Only a polynomial number of sub-problems occurs in total.

- **Memoization (top down):**
  - Apply standard recursion, but remember the solution to a previously solved sub-problem.
  - Re-use solution whenever a sub-problem is encountered that has already been solved.
- **Tabulation (bottom up):**
  - Build a table of solutions for the sub-problems in bottom-up fashion.
- **Complexity:** Roughly, we get the number of sub-problems times the complexity for solving every sub-problem.

Dynamic Programming: Matrix Chain Multiplication

- The standard method for multiplying a $p \times q$ matrix with a $q \times r$ matrix requires $p \cdot q \cdot r$ (scalar) multiplications and $p \cdot (q-1) \cdot r$ additions, yielding a $p \times r$ result matrix.
- Recall that matrix multiplication is associative, but not commutative:

$$(\mathbf{A} \cdot \mathbf{B}) \cdot \mathbf{C} = \mathbf{A} \cdot (\mathbf{B} \cdot \mathbf{C}) \quad \text{but, in general,} \quad \mathbf{A} \cdot \mathbf{B} \neq \mathbf{B} \cdot \mathbf{A}.$$

- Hence, if $\mathbf{A}$ is a 100×1 matrix, $\mathbf{B}$ is a 1×100 matrix, and $\mathbf{C}$ is a 100×1 matrix, then
  - $(\mathbf{A} \cdot \mathbf{B}) \cdot \mathbf{C}$ needs $(100 \cdot 1 \cdot 100) + (100 \cdot 100 \cdot 1) = 20\,000$ multiplications.
  - $\mathbf{A} \cdot (\mathbf{B} \cdot \mathbf{C})$ needs $(1 \cdot 100 \cdot 1) + (100 \cdot 1 \cdot 1) = 200$ multiplications!
- It is obvious that it may pay off to think about an optimal parenthesization.

Problem: MATRIXCHAINMULTIPLICATION

Input: A sequence of n matrices $\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_n$, where matrix $\mathbf{A}_i$ has dimensions $d_{i-1} \times d_i$ for $i \in \{1, 2, \ldots, n\}$.

Output: An optimal parenthesization such that the standard computation of $\mathbf{A}_1 \cdot \mathbf{A}_2 \cdot \ldots \cdot \mathbf{A}_n$ results in the minimum number of multiplications.

Dynamic Programming: Matrix Chain Multiplication

- We can split the product of matrices into two products by multiplying the first k matrices, multiplying the second $n-k$ matrices, and then multiplying the two resulting matrices:

$$\mathbf{A}_1 \cdot \mathbf{A}_2 \cdot \ldots \cdot \mathbf{A}_n = (\mathbf{A}_1 \cdot \ldots \cdot \mathbf{A}_k) \cdot (\mathbf{A}_{k+1} \cdot \ldots \cdot \mathbf{A}_n)$$

  Of course, k can be any number out of $\{1, 2, \ldots, n-1\}$.

Optimality Observation

If an optimal solution for $\mathbf{A}_i \cdot \ldots \cdot \mathbf{A}_j$ is given by $(\mathbf{A}_i \cdot \ldots \cdot \mathbf{A}_k) \cdot (\mathbf{A}_{k+1} \cdot \ldots \cdot \mathbf{A}_j)$, for $1 \leq i \leq k < j \leq n$, then also the parenthesizations of $\mathbf{A}_i \cdot \ldots \cdot \mathbf{A}_k$ and $\mathbf{A}_{k+1} \cdot \ldots \cdot \mathbf{A}_j$ need to be optimal.

Dynamic Programming: Matrix Chain Multiplication

- For $1 \le i \le j \le n$, let $m[i,j]$ denote the minimum number of scalar multiplications needed to compute $\mathbf{A}_i \cdot \ldots \cdot \mathbf{A}_j$.
- Recall that $\mathbf{A}_i$ has dimensions $d_{i-1} \times d_i$. Hence, for $i \le k < j$,

$$\underbrace{(\mathbf{A}_i \cdot \ldots \cdot \mathbf{A}_k)}_{d_{i-1} \times d_k} \cdot \underbrace{(\mathbf{A}_{k+1} \cdot \ldots \cdot \mathbf{A}_j)}_{d_k \times d_j} \qquad \text{has dimensions } d_{i-1} \times d_j.$$

- We get the following formula:

$$m[i,j] = \begin{cases} 0 & \text{if } i = j, \\ \min_{i \le k < j}\{m[i,k] + m[k+1,j] + d_{i-1} d_k d_j\} & \text{if } i < j. \end{cases}$$

- As in the case of the Fibonacci numbers, a naïve evaluation of this recursive formula would result in re-computing partial solutions over and over again.
- We resort to dynamic programming, and tabulate $m[i,j]$ as it becomes known.
- In the pseudo code on the next slide, we use $s[i,j]$ to store the optimum value of k for splitting $\mathbf{A}_i \cdot \ldots \cdot \mathbf{A}_j$ into $(\mathbf{A}_i \cdot \ldots \cdot \mathbf{A}_k) \cdot (\mathbf{A}_{k+1} \cdot \ldots \cdot \mathbf{A}_j)$.
- The dimensions of $\mathbf{A}_1, \mathbf{A}_2, \ldots, \mathbf{A}_n$ are stored in the array $d[]$.

Dynamic Programming: Matrix Chain Multiplication

```
void MatrixChainMultiplication(int d[], int s[])
{
   int seq_len, cost;
   int N = d.length - 1;
   for (i = 1; i <= N; i++)    m[i, i] = 0;
   for (seq_len = 2;  seq_len <= N;  ++seq_len) {
      for (i = 1;  i <= N - seq_len + 1;  ++i) {
         j = i + seq_len - 1;
         m[i, j] = MAX_INT;       // "infinity"
         for (k = i;  k <= j - 1;  ++k) {
            cost = m[i, k] + m[k+1, j] +
                   d[i-1] * d[k] * d[j];
            if (cost < m[i, j]) {
               m[i, j] = cost;  // minimum cost so far
               s[i, j] = k;     // index of best split
            }
         }
      }
   }
}
```

Dynamic Programming: Matrix Chain Multiplication

- It is an easy exercise to extract the actually best parenthesization from $s[]$:

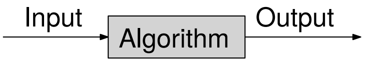
```
string GetParenthesization(int i, int j, int s[])
{
   if (i < j) {
      x = GetParenthesization(i, s[i,j], s);
      y = GetParenthesization(s[i,j] + 1, j, s);
      return "(x * y)";
   }
   else
      return "A_" # IntToString(i);
}
```

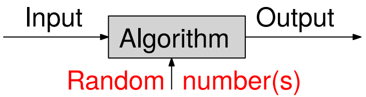
- Hence we get the following result:

Theorem 84

MatrixChainMultiplication can be solved in $O(n^3)$ time and $O(n^2)$ space for n matrices.

Deterministic vs. Randomized Algorithm





Deterministic algorithm:

- It will always produce the same output in repeated runs for a particular input.
- The underlying state machine will always pass through the same sequence of states for the same input.
- Differences in running time for the same input are small and due to system-dependent reasons.

Randomized algorithm:

- It uses a random number at least once to make a (branching) decision.
- Repeated runs for the same input may result in different outputs and/or running times.
- Probability of generating incorrect output.
- Efficiency is guaranteed only with some probability.

- Randomization and probabilistic methods play a key role in modern algorithm theory: Randomized algorithms are often simpler to understand and implement, while being correct and efficient with high probability.

Randomization: Random Numbers

- "Classical" approaches like the rolling of dice or the flipping of coins cannot be used by computers.
- One alternative is to measure some physical phenomenon that can be expected to be random. E.g., the seconds of the current wall-clock time can be expected to yield a random number between 0 and 59.
- Most Unix/Linux-like operating systems have `/dev/urandom`, which allows to access environmental noise collected from sources like device drivers.
- The second alternative is to use an algorithm to generate [sic!] random numbers: pseudorandom number generator (PRNG).
- E.g., `arc4random()` is available on BSD platforms, and also on GNU/Linux with `libbsd`. It is an easy-to-use option for most standard C/C++-applications that is much better than `rand()`. The `rand48()` family is better than `rand()`, too!

Practical advice

- Invest more time into testing since achieving path coverage becomes trickier!
- Employ randomization in such a way that the algorithm's behavior can be made reproducable — i.e., deterministic! — if required: Debugging might be needed!

Randomization: Random Numbers in C

- The following code generates a pseudorandom integer within the set $\{from, \ldots, to\}$.

```c
int RandomNumberRange(const int from, const int to)
{
   int rnd, range = to - from + 1;
   int maxSafeRange = maxRndNumber - (maxRndNumber % range);

   do {
      rnd = GetRandomNumber();  // e.g., use arc4random()
   } while (rnd >= maxSafeRange);

   return from + (rnd % range);
}
```

- Note that solutions simply resorting to the modulo operator, %, to restrict a random number to a range of numbers tend to produce skewed results.
- The skew in the distribution is made worse if the random number is obtained from an LCG since LCGs (like `rand()`) tend to have poor entropy in the lower bits.

Randomization: Random Numbers in C++

```
#include <random>

std::random_device  rnd_dev;
std::mt19937        gen(rnd_dev());

int RandomNumberRange(const int from, const int to)
{
   std::uniform_int_distribution<int>  distr(from, to);
   return distr(gen);
}
```

- The class `std::random_device` is a uniformly-distributed integer random number generator that makes use of a non-deterministic source if it is available.
- We use it to seed a Mersenne Twister PRNG based on the Mersenne prime $2^{19937} - 1$, which has a period of $2^{19937} - 1$.
- Then this PRNG is used to generate a 32-bit random number, which is mapped to the set $\{from, \dots, to\}$ via a call to `std::uniform_int_distribution`.
- Use `rand()` instead of `std::random_device`, together with `srand()`, for a seeding of `std::mt19937` that yields reproducable results.
- The STL also contains a 64-bit implementation: `std::mt19937_64`.

Randomization: Monte Carlo vs. Las Vegas

Monte Carlo algorithm:

- Is always fast.
- Might fail to produce a correct output, with one-sided or two-sided errors.
- The probability of an incorrect output is bound based on an error analysis.
- Repetitions of Monte Carlo algorithms tend to drive down the failure probability exponentially.

Las Vegas algorithm:

- Always gives a correct output (or reports an error).
- Its run-time performance may vary.

- Several Las Vegas algorithms can be turned into Monte Carlo algorithms by setting a time budget and stopping the algorithm once this time budget is exceeded.

Random Permutation

Problem: RANDOMPERMUTATION

Input: A sequence $S = (s_0, s_1, \ldots, s_{n-1})$ of n entities.

Output: A random permutation of these n entities, uniformly at random.

```
void RandomPermutation(array S[]) // Knuth shuffle of S[0:N]
{
   N = length(S);
   for (i = N;  i >= 1;  --i) {
      j = RandomInteger({0,1,...,i});
      Swap(S[i], S[j]);
   }
}
```

- Knuth's version of the Fisher-Yates shuffle [1938] runs in $\Theta(n)$ time, with $n := |S|$.
- After `RandomPermutation(S)` we have $\Pr[s = s_i] = {}^1/_n$ for all $s \in S$ and all $i \in \{0, 1, \ldots, n-1\}$.
- Hence `RandomPermutation(S)` generates each permutation with probability ${}^1/_{n!}$, i.e., uniformly at random.

Randomized QuickSort

- We assume that all numbers of the array to be sorted are distinct.

Standard QuickSort:

1. Pick the left-most element p of the array as the pivot.
2. Rearrange and split the array into two subarrays LESS and GREATER by comparing each element to p.
3. Recurse on LESS and GREATER.

- $O(n^2)$ worst-case complexity, even when using median-of-three partitioning.
- One can specify worst-case input!
- $O(n \log n)$ average-case complexity.

Randomized QuickSort:

1. Pick an element p of the array as the pivot, uniformly at random.
2. Rearrange and split the array into two subarrays LESS and GREATER by comparing each element to p.
3. Recurse on LESS and GREATER.

- $O(n \log n)$ expected-time complexity for all inputs of n numbers.
- One can also generate a random permutation of the input numbers and then run the standard QuickSort on that shuffled array.

Randomized QuickSort

Theorem 85

The expected number of comparisons made by a randomized QuickSort on an array of n input numbers is at most $2n \ln n$.

Proof: We define the random variable X_{ij} to be 1 if the algorithm does compare the i-th smallest element to the j-th smallest element, and 0 otherwise.
Let X denote the total number of comparisons. Since we never compare the same pair of elements twice, we get

$$X = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} X_{ij},$$

and, due to the linearity of the expectation (Lemma 24),

$$\mathbb{E}(X) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \mathbb{E}(X_{ij}).$$

Consider X_{ij} for $1 \leq i < j \leq n$. We denote the i-th smallest element in the array by e_i and the j-th smallest element by e_j.

Randomized QuickSort

Proof of Theorem 85 (cont'd) :

1. If we choose a pivot p such that $e_i < p < e_j$ then e_i ends up in LESS and e_j ends up in GREATER, and e_i and e_j will never be compared.
2. If we choose e_i or e_j as pivot then we do compare them.
3. If we choose $p < e_i$ or $p > e_j$ then the decision is deferred, and we will pick a new pivot in the next recursive step.

At each step, the probability that $X_{ij} = 1$ under the condition that we will certainly not compare e_i to e_j in the future is exactly $^2/_{j-i+1}$. Hence, the overall probability of $X_{ij} = 1$ equals $^2/_{j-i+1}$, too.
Recall Lemma 9 on the Harmonic numbers H_n. We get

$$\mathbb{E}(X) = \sum_{i=1}^{n-1} \sum_{j=i+1}^{n} \mathbb{E}(X_{ij}) = \sum_{i=1}^{n-1} 2 \sum_{j=i+1}^{n} \frac{1}{j-i+1} = \sum_{i=1}^{n-1} 2 \left(\frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{n-i+1} \right)$$

$$< 2n \left(\frac{1}{2} + \frac{1}{3} + \ldots + \frac{1}{n} \right) = 2n \cdot (H_n - 1) \leq 2n \ln n.$$

□

Average case versus expected case

Since we average over all permutations (of some particular input!), this $O(n \log n)$ bound is a *worst-case expected-time* bound and applies even to (mostly) sorted input!

Randomized Primality Testing

Problem: PRIME

Input: A natural number n with $n > 1$.

Decide: Is n prime? I.e., can n be divided only by 1 and by itself?

- Note that we only care to know whether some number n is prime; we do not seek a prime factorization of n.
- PRIME is a basic building block for many applications. E.g., large primes are frequently sought in cryptography.
- Brute-force methods — e.g., repeated divisions by $2, 3, \ldots, \lfloor\sqrt{n}\rfloor$ — are far too slow when n is truly large. (Exponential worst-case running time in the size of n.)
- PRIME is solvable in polynomial time [Agrawal&Kayal&Saxena (2002)]: Their algorithm runs in $O(\log^{7.5+\varepsilon} n)$ time, which is polynomial in the size of n. (In 2005, Pomerance&Lenstra reduced this to $O(\log^{6+\varepsilon} n)$.)
- But this is a rather theoretical result . . .
- Fortunately, large primes are not particularly rare.
- Expectation: One out of $\ln n$ random integers of the size of n will be prime!
- Randomization yields an efficient, simple and easy-to-implement primality test — if we accept a small probability of error!

Randomized Primality Testing: Basic Idea

Witness of compositeness

Find a predicate P and a suitable set S (with, typically, $S \subseteq \mathbb{N}$) such that

$$p \in \mathbb{P} \quad \Rightarrow \quad (\forall s \in S \;\; P(s,p))\,.$$

This is equivalent to

$$(\exists s \in S \;\; \neg P(s,p)) \quad \Rightarrow \quad p \notin \mathbb{P}.$$

- Suppose that $p \notin \mathbb{P}$ and that $\neg P(s,p)$ holds for, say, at least 50% of the elements $s \in S$.
- Then we incorrectly classify a number p as prime
  - after testing $P(s,p)$ for just one $s \in S$ with a probability of at most $^1/_2$;
  - after testing $P(s,p)$ for just two $s \in S$ with a probability of at most $^1/_4$;
  - after testing $P(s,p)$ for k numbers of S with a probability of at most $^1/_{2^k}$.

Randomized Primality Testing: Fermat

Lemma 86 (*Fermat's Little Theorem, Dt.: Kleiner Satz von Fermat*)

If $p \in \mathbb{P}$ then $a^p \equiv_p a$ for every $a \in \mathbb{N}$.

- If a is not a multiple of p then this reduces to $a^{p-1} \equiv_p 1$.
- Hence, if $a^{n-1} \not\equiv_n 1$ for a given $n \in \mathbb{N}$ and some $a \in \{2, 3, \ldots, n-1\}$ then n is composite, i.e., not a prime.
- Such an integer a is called a *Fermat witness* for the compositeness of n.
- Otherwise, n is possibly prime — or a is a so-called *Fermat liar*.
- E.g., $2^{242} \bmod 243 = 121$, implying that 243 is composite. And, indeed $243 = 3^5$.
- E.g., $2^{240} \bmod 241 = 1$, implying that 241 could be prime. And, indeed, 241 is prime.

Randomized Primality Testing: Fermat

- However, $2^{560} \bmod 561 = 1$, but $561 = 3 \cdot 11 \cdot 17$.
- Worse, $4^{560} \bmod 561 = 1$ and $5^{560} \bmod 561 = 1$ and $7^{560} \bmod 561 = 1$ and $8^{560} \bmod 561 = 1$ and ...
- We have $a^{560} \bmod 561 = 1$ for all $a \in \{2, 3, \ldots, 560\}$ for which $\gcd(561, a) = 1$. The number 561 is the smallest so-called *Carmichael number*.
- Carmichael numbers are rather rare: There are about $2 \cdot 10^7$ Carmichael numbers between 1 and 10^{21}, i.e., on average one Carmichael number within $5 \cdot 10^{13}$ numbers. (But there are infinitely many Carmichael numbers.)

Lemma 87

If n is a composite number that is no Carmichael number then at least half of all $a \in \{2, 3, \ldots, n-2\}$ are Fermat witnesses.

Theorem 88

If n is a composite number that is no Carmichael number then k rounds of the Fermat primality test (with k randomly chosen values for $a \in \{2, 3, \ldots, n-2\}$) will incorrectly classify n as prime with probability at most 2^{-k}.

Randomized Primality Testing: Fermat

```
bool IsPrimeFermat(int n, int k)
{
   A = {2,3,...,n-2};
   for (i = 1;  i <= k;  ++i) {
      a = RandomInteger(A);
      if (gcd(n, a) != 1)     return false; /* composite */
      if ((a^(n-1) % n) != 1) return false; /* composite */
      A = A \ {a};
   }
   return true;  /* probably prime */
}
```

- `IsPrimeFermat` is a Monte Carlo algorithm with one-sided error: it will classify all primes as “prime”, and falsely report a composite number as “prime” with probability at most 2^{-k}. That is, it is correct with high probability.
- Note that the number k of random trials need not be scaled with the size of n in order to keep the error probability below 2^{-k}.
- Still, the Fermat primality test is not considered to be reliable enough on its own grounds. It is, however, used for a rapid screening of possible candidate primes.

Randomized Primality Testing: Miller-Rabin

Lemma 89

Let $n \in \mathbb{N}$ be prime with $n > 2$, and $s, d \in \mathbb{N}_0$ such that $n - 1 = 2^s \cdot d$, with d odd. Then for all $a \in \{2, 3, \ldots, n-2\}$ we have

$$a^d \equiv_n 1 \qquad \text{or} \qquad a^{2^r \cdot d} \equiv_n -1 \quad \text{for some } r \in \{0, 1, \ldots, s-1\}.$$

- The contrapositive of this lemma yields a test for compositeness:

Lemma 90

Let $n \in \mathbb{N}$ be odd with $n \geq 5$, and $s, d \in \mathbb{N}_0$ such that $n - 1 = 2^s \cdot d$, with d odd. If there exists an $a \in \{2, 3, \ldots, n-2\}$ such that

$$a^d \not\equiv_n 1 \qquad \text{and} \qquad a^{2^r \cdot d} \not\equiv_n -1 \quad \text{for all } r \in \{0, 1, \ldots, s-1\},$$

then n is composite.

- Such an integer a is called an *MR-witness* of compositeness.

Randomized Primality Testing: Miller-Rabin

```
bool IsPrimeMillerRabin(int n, int k)   /* for odd n > 2 */
{
   s = 0;  d = n - 1;
   while (IsEven(d)) { /* (n-1) = 2^s*d with odd d */
      ++s;  d /= 2;
   }
   A = {2,3,...,n-2};
 LOOP: for (i = 1;  i <= k;  ++i) {
      a = RandomInteger(A);  A = A \ {a};
      x = a^d % n;
      if ((x == 1)  ||  (x == -1)) do next LOOP;
      for (j = 1;  j < s;  ++j) {
         x = x^2 % n;
         if (x ==  1) return false; /* composite */
         if (x == -1) do next LOOP;
      }
      return false; /* composite */
   }
   return true;  /* probably prime */
}
```

Randomized Primality Testing: Miller-Rabin

Lemma 91

Let $n \in \mathbb{N}$ be an odd composite number with $n \geq 5$. Then the set $\{2, 3, \ldots, n-2\}$ contains at most $\frac{n-3}{4}$ numbers a such that $\gcd(n, a) = 1$ but a is no MR-witness of the compositeness of n.

- Trivially, if $\gcd(n, a) > 1$ then a is always a witness of the compositeness of n.

Theorem 92 (*Miller (1976), Rabin (1980)*)

If n is an odd composite number then the Miller-Rabin primality test with k rounds (and k randomly chosen values for $a \in \{2, 3, \ldots, n-2\}$) will incorrectly classify n as prime with probability at most 4^{-k}.

- Hence, 10 rounds of the Miller-Rabin primality test give us a probability of error that is $4^{-10} \approx 10^{-6}$, and 20 rounds result in a probability of error that is roughly 10^{-12}. After 30 rounds we are down to roughly 10^{-18} error probability.
- For comparison purposes: Quality hard disks have a probability of about 10^{-16} for an unrecoverable read error (URE).
- Note that this error bound does not depend on the size of n and that it holds also for Carmichael numbers!

Randomized Primality Testing: Miller-Rabin

Lemma 93

One round of the Miller-Rabin primality test for input number n takes $O(\log^3 n)$ time when using modular exponentiation by repeated squaring.

- FFT-based multiplication can bring the time complexity of one round down to $O(\log^2 n \cdot \log(\log n) \cdot \log(\log(\log n)))$.
- If the Generalized (aka Extended) Riemann Hypothesis (GRH) — which is a number-theoretic conjecture that is generally believed to be true — holds then for every composite number n the set $\{1, 2, \dots, \lfloor 2 \ln^2 n \rfloor\}$ contains an MR-witness for n. Hence, if one assumes the Extended Riemann Hypothesis then there is a deterministic algorithm to test primality in time $O(\log^5 n)$.
- [Jiang&Deng (2014)]: If n is "small" then smaller sets of potential MR-witnesses are known, with no need to resort to the GRH:
  - If $n < 2^{11} - 1 = 2047$: It suffices to test $a \in \{2\}$.
  - If $n < 2^{64}$: It suffices to test $a \in \{2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37\}$.
- [Sorenson&Webster (2015)] go even beyond 64-bit results:
  - If $n < 10^{24}$: It suffices to test $a \in \{2, 3, 5, 7, 11, 13, 17, 19, 23, 29, 31, 37, 41\}$.

Linear-Time Selection

Definition 94 (*Order statistic, Dt.: Ordnungsstatistik*)

Consider a finite (totally-ordered) set S of n distinct elements and a number k, for $k, n \in \mathbb{N}$. An element $x \in S$ is the *k-th smallest element* of S, aka the *k-th order statistic*, if $|\{s \in S : s < x\}| = k - 1$. If $k = \lceil \frac{n}{2} \rceil$ then the k-th smallest element of S is also called the *median* of S.

Problem: SELECTION

Input: A set S of n distinct (real) numbers and a number k, for $k, n \in \mathbb{N}$.

Output: The k-th smallest element of S.

- If $k = 1$ or $k = n$ then SELECTION can be solved easily using $n - 1$ comparisons.
- If the numbers of S are arranged in sorted order then the k-th smallest element can be found in $O(n)$ time. (Or even faster.)
- What about general values of k and unsorted numbers?

Theorem 95 (*Blum&Floyd&Pratt&Rivest&Tarjan (1973)*)

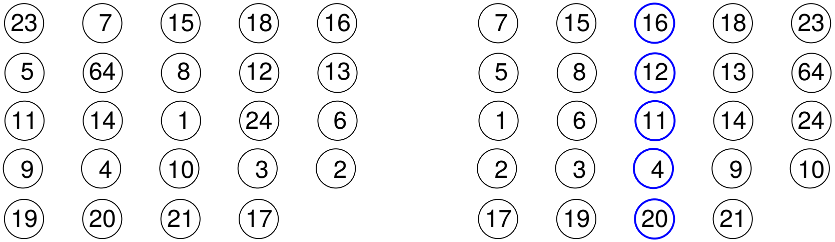
SELECTION among n distinct numbers can be solved in $O(n)$ time, for any $n, k \in \mathbb{N}$.

Linear-Time Selection

Proof of Theorem 95 :

1. Divide the n elements of S into $\lfloor n/5 \rfloor$ groups of 5 elements each and (at most) one group containing the remaining $n \bmod 5$ elements.
2. Sort each group and compute its median.

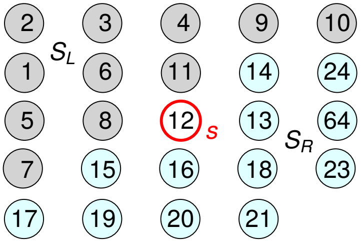
- Suppose that we want to compute the k-th smallest element of $S := \{23, 7, 15, 18, 16, 5, 64, 8, 12, 13, 11, 14, 1, 24, 6, 9, 4, 10, 3, 2, 19, 20, 21, 17\}$, for $k := 7$ and $n := |S| = 24$.

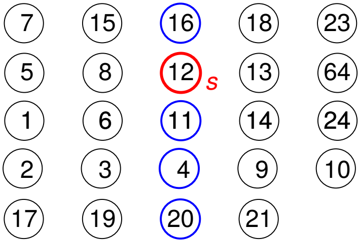


Linear-Time Selection

Proof of Theorem 95 :

1. Divide the n elements of S into $\lfloor n/5 \rfloor$ groups of 5 elements each and (at most) one group containing the remaining $n \bmod 5$ elements.
2. Sort each group and compute its median.
3. Recursively find the median s of the $\lceil n/5 \rceil$ medians found in the previous step.
4. Partition S relative to the median-of-medians s into S_L and S_R (and $\{s\}$) such that all elements of S_L are smaller than s and all elements of S_R are greater than s.
5. Let $m := |S_L \cup \{s\}|$. If $k = m$ then return s. Otherwise, if $k < m$ then recurse on S_L to find the k-th smallest element, else (if $k > m$) recurse on S_R to find the $(k - m)$-th smallest element.





Linear-Time Selection

Proof of Theorem 95 (cont'd) :

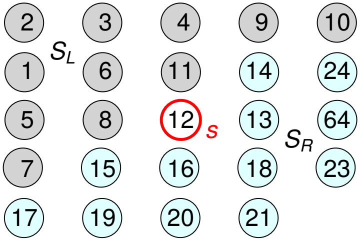
- What is the complexity of MedianOfMedians? We get

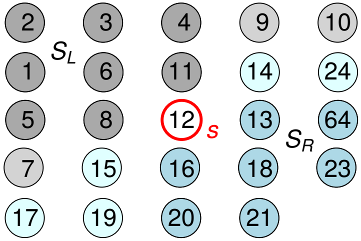
$$m = |S_L| + 1 \geq 3 \left\lceil \frac{1}{2} \lceil n/5 \rceil \right\rceil \geq \frac{3}{10} n, \qquad \text{and, thus, } |S_L| \geq \frac{3}{10} n - 1.$$

- Hence, $|S_R| \leq \frac{7}{10} n$. Similarly, $|S_R| \geq \frac{3}{10} n + O(1)$ and $|S_L| \leq \frac{7}{10} n + O(1)$, resulting in the currence relation

$$T(n) \leq T\left(\frac{n}{5}\right) + T\left(\frac{7n}{10}\right) + O(n), \quad \text{which yields } T \in O(n).$$

□





Linear-Time Selection

- Unfortunately, the constant hidden in the O-term is fairly large: Depending on details of the actual implementation, this algorithm requires about $50n$ comparisons!
- Hence, this form of linear-time selection is too slow to be useful in practice.
- [Alexandrescu (SEA 2017)]: MedianOfNinthers, which is a refined version of MedianOfMedians, is a linear-time selection scheme that works decently in practice.
- What about randomization? We could pick an element of S randomly and regard it as the median of medians . . .

Expected Linear-Time Selection

1. Pick an element s *uniformly at random* from S.
2. Partition S relative to s into S_L and S_R (and $\{s\}$) such that all elements of S_L are smaller than s and all elements of S_R are greater than s.
3. Let $m := |S_L \cup \{s\}|$. If $k = m$ then return s. Otherwise, if $k < m$ then recurse on S_L to find the k-th smallest element, else (if $k > m$) recurse on S_R to find the $(k - m)$-th smallest element.

What is the complexity of this randomized algorithm?

Worst case: If s is the smallest or largest element of S then S shrinks by only one element, and we get $O(n^2)$ complexity.
The probability of consistently picking an element of S which currently is the smallest or largest is

$$\frac{2}{n} \cdot \frac{2}{n-1} \cdot \frac{2}{n-2} \cdot \ldots \cdot \frac{2}{3} \cdot \frac{2}{2} = \frac{2^{n-1}}{n!}.$$

Best case: The element s turns out to be the k-th smallest element, with probability ${}^1/_n$.

Expected Linear-Time Selection

Expected complexity:

- Let $T(n)$ be an upper bound on the expected time to process a set S with n (or fewer) elements.
- Call s lucky if $|S_L| \leq {}^{3n}\!/_4$ and $|S_R| \leq {}^{3n}\!/_4$.
- Hence, s is lucky if it lies betwen the 25th and the 75th percentile of S, which happens with probability ${}^1\!/_2$.
- This gives us

$$\begin{aligned} T(n) &\leq \text{(time to partition)} + \text{(maximum expected time for recursion)} \\ &\leq n + \Pr(s \text{ is lucky}) \cdot T\left(\frac{3n}{4}\right) + \Pr(s \text{ is unlucky}) \cdot T(n) \\ &= n + \frac{1}{2} T\left(\frac{3n}{4}\right) + \frac{1}{2} T(n). \end{aligned}$$

- Hence, after subtracting $\frac{1}{2}T(n)$ from both sides, we get

$$T(n) \leq T\left(\frac{3n}{4}\right) + 2n, \quad \text{i.e., } T(n) \leq 8n.$$

Theorem 96

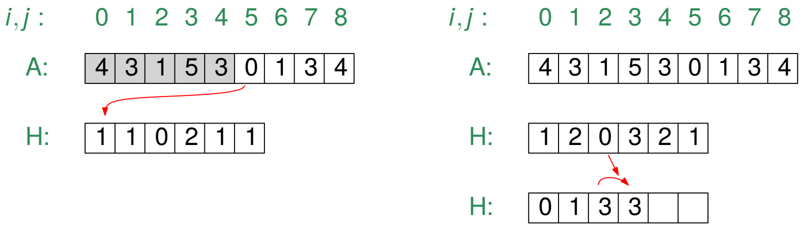
A simple randomized algorithm solves SELECTION in expected linear time.

Counting Sort

- Counting Sort can be used for sorting an array A of n elements whose keys are integers within the range $[0, k-1]$, for some $n, k \in \mathbb{N}$.
- It is stable but not in-place.
- It uses indices into an array and, thus, is not a comparison sort.

Basic idea:

1. Compute a histogram H of the number of times each element occurs within A.
2. For all possible keys, do a prefix sum computation on H to compute the starting index in the output array of the elements which have that key.



Counting Sort

Basic idea:

3. Move each element to its sorted position in the output array B.

i, j :	0	1	2	3	4	5	6	7	8
A:	4	3	1	5	3	0	1	3	4
H:	0	1	3	3	6	8			
B:									

i, j :	0	1	2	3	4	5	6	7	8
A:	4	3	1	5	3	0	1	3	4
H:	0	2	3	5	7	9			
B:		1		3	3		4		5

Theorem 97

Counting Sort is a stable sorting algorithm that sorts an array of n elements whose keys are integers within the range $[0, k-1]$, for some $n, k \in \mathbb{N}$, within $O(n+k)$ time and space.

Counting Sort

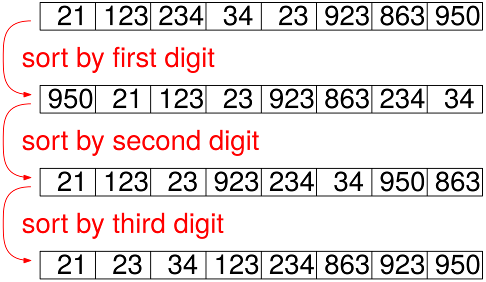
```
CountingSort(array A[], array B[], array H[], int n, int k)
{
   /* calculate histogram */
   for (i = 0;  i < k;  ++i)  H[i]      = 0;
   for (j = 0;  j < n;  ++j)  H[A[j]] += 1;
   /* calculate the starting index for each key */
   total = 0;
   for (i = 0;  i < k;  ++i) {
      oldCount = H[i];
      H[i]     = total;
      total   += oldCount;
   }
   /* stable copy to output array */
   for (j = 0;  j < n;  ++j) {
      B[H[A[j]]] = A[j];
      H[A[j]]   += 1;
   }
}
```

Radix Sort

- Radix Sort can be used for sorting an array A of n elements whose keys are d-digit (non-negative) integers, for some $n, d \in \mathbb{N}$.
- It compares keys on a per-digit basis and, thus, is not a comparison sort.
- It is stable but not in-place.

Basic idea:

1. Use a stable sorting algorithm to sort the elements relative to the least significant digit of their keys.
2. Then sort on the second least-significant digit, and so on.



Radix Sort: Complexity

```
RadixSort(array A[], int n, int d)
{
    /* digit 1 is least significant,
       digit d is most significant */
    for (i = 1;  i <= d;  ++i) {
       use stable sort to sort A[] relative to digit i
    }
}
```

Theorem 98

Radix Sort is a stable sorting algorithm that can be implemented to sort an array of n elements whose keys are formed by the Cartesian product of d digits, with each digit out of the range $[0, k-1]$, within $O(d(n+k))$ time and $O(n+k)$ space, for $n, d, k \in \mathbb{N}$.

Proof: The correctness can be established by induction. If Counting Sort is used for sorting according to the i-th digit then $O(n+k)$ time is consumed per digit. □

- It is obvious that Radix Sort can be employed whenever keys are to be sorted lexicographically such that each key is formed by the Cartesian product of “digits”, where each digit belongs to some (ordered) finite set.

Radix Sort: Discussion

- Whether or not Radix Sort is faster than comparison-based sorting algorithms depends on the assumptions made.
- If we regard an integer as a word with w bits then Theorem 98 implies that Radix Sort runs in $O(w \cdot n)$ time, i.e., in time linear in n if w is assumed to be constant.
- However, w can hardly be considered a constant: if all n keys are distinct, then w has to be at least $\log n$ for a RAM to be able to store them in memory, resulting in a time complexity of $\Omega(n \log n)$.
- The $O(n \log n)$ bound on the worst-case time complexity of optimal comparison-based sorting algorithms holds only if constant time per comparison can be assumed.
- If w cannot be assumed to be constant then this assumption is weak, too: Comparisons of randomly generated keys take constant time on average because keys differ on the very first bit in half the cases, and differ on the second bit in half of the remaining half, etc. However, in a sorting algorithm the keys cannot be regarded as random as the sort progresses!
- Radix Sort can only sort according to a lexicographical ordering, while comparison-based sorting algorithms are more general. But this tends to be of little importance in practice.

Priority Queues

Binomial Heaps

Fibonacci Heaps

Abstract Data Type: Priority Queue

Priority Queue (Dt.: Vorrangwarteschlange)

A *priority queue* (PQ) is an ADT that arranges data elements according to per-element keys ("priorities"): In a minimizing (maximizing, resp.) PQ the element with smallest (largest, resp.) overall key is served first.

- Keys need to belong to a totally ordered set.
- Standard operations for minimizing PQs:
  - FindMin: return element with smallest key,
  - DeleteMin: return and remove element with smallest key from PQ,
  - Insert: insert a new element,
  - DecreaseKey: decrease the key of an element,
  - Remove: remove an element from PQ,
  - Merge: merge (aka meld) two PQs.

- Standard implementation of PQ: binary heap.
  - FindMin in $O(1)$.
  - Insert, DeleteMin, Remove and DecreaseKey in $O(\log n)$ time if heap has n elements.
  - Merge in $O(n_1 + n_2)$ time for two heaps with n_1 and n_2 elements.

Binomial Tree

Definition 99 (*Binomial tree, Dt.: Binomialbaum*)

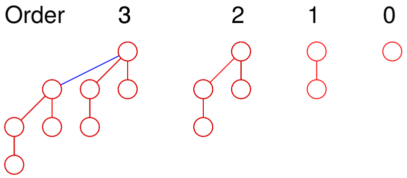
A *binomial tree* is a rooted and ordered tree which is defined recursively as follows:

- A binomial tree of order 0 consists only of the root node;
- For $k \in \mathbb{N}_0$, a binomial tree of order $k+1$ consists of two binomial trees of order k such that one binomial tree is the left-most subtree of the other.

Lemma 100

For $k \in \mathbb{N}_0$, a binomial tree of order k has k subtrees (from left to right) of orders $k-1, k-2, \ldots, 1, 0$.

Proof : By induction on k. □



Lemma 101

For $k \in \mathbb{N}_0$, a binomial tree of order k has 2^k nodes and height k.

Lemma 102

For $k \in \mathbb{N}_0$, a binomial tree of order k has $\binom{k}{d}$ nodes at depth d.

Binomial Heap

Definition 103 (*Binomial heap*)

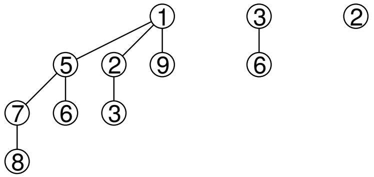
A *binomial heap* is a collection of binomial trees that satisfy the *binomial heap property*:

- Each binomial tree is a minimizing heap, i.e., for all nodes v of the binomial tree, all keys of the children of v are greater than (or at most equal to) the key of v.
- For any $k \in \mathbb{N}_0$, there is at most one binomial tree of order k.
- The binomial trees are arranged in a right-to-left sorted sequence according to their orders, with the tree of smallest order being right-most.

Lemma 104

For $n \in \mathbb{N}_0$, a binomial heap with a total of n nodes contains a binomial tree of order k if and only if the bit that corresponds to 2^k in the binary representation of n is 1.

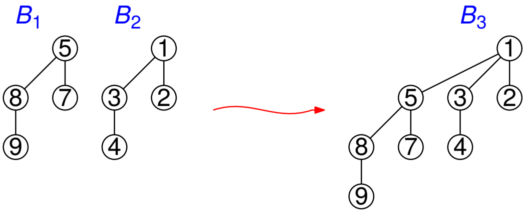
Proof: Recall Lem. 101, and that the binary representation of $n \in \mathbb{N}_0$ is unique. □



- E.g., $11 = 2^3 + 2^1 + 2^0 = (1011)_2$.

Binomial Heap: Merging in a Special Case

- Suppose that we want to merge two binomial heaps in the special case that both heaps contain only one binomial tree of the same order k. Let B_1 and B_2 be these two trees.
- We generate one binomial tree B_3 of order $k+1$ by making B_1 the left-most child of B_2 if the key of the root of B_2 is less than the key of the root of B_1. Otherwise, B_2 becomes the left-most child of B_1.



- Recap: How do we add numbers in binary representation?
- E.g., lets add $n_1 := 5 = (0101)_2$ and $n_2 := 7 = (0111)_2$. We should get $12 = (1100)_2$.

n_1:	0	1	0	1
n_2:	0	1	1	1
carry:	1	1	1	–
result:	1	1	0	0

Binomial Heap: Merging

Merging Binomial Heaps

- We visit the binomial trees of both binomial heaps according to increasing order k, starting with $k := 0$.
- If both heaps and the carry contain exactly …
  - … no binomial tree of order k: Do nothing.
  - … one binomial tree B_1 of order k: move B_1 to the result.
  - … two binomial trees B_1, B_2 of order k: Merge B_1 and B_2 into a tree B of order $k+1$ and move B to the carry.
  - … three binomial trees B_1, B_2, B_3 of order k: Merge B_1 and B_2 into a tree B of order $k+1$ and move B to the carry; move B_3 to the result.
- Increment k after processing the binomial trees of order k.

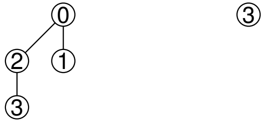
Lemma 105

Merging two binomial heaps with a total of n nodes takes $O(\log n)$ time.

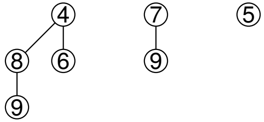
Proof: Lemma 104 implies that a binomial heap with i nodes contains at most $\lfloor \log(i) \rfloor + 1$ binomial trees. Hence, we need to perform $O(\log n)$ trivial merges of two binomial trees of the same order. Each such merge takes $O(1)$ time. □

Binomial Heap: Merging

binomial heap I:

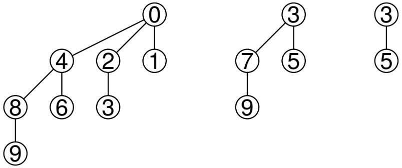


binomial heap II:

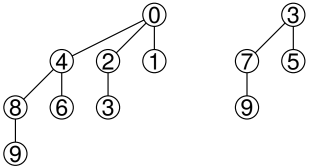


carry:

$k = 3$



merged heap:



Binomial Heap: Other Operations

Lemma 106

> A new element can be inserted into a binomial heap with a total of n nodes in $O(\log n)$ worst-case and $O(1)$ amortized time.

Proof : We create a new heap that contains only the new element and merge it with the old heap. The amortized analysis is similar to the one used for incrementing a binary counter. □

Lemma 107

> Finding the minimum element in a binomial heap with a total of n nodes takes $O(\log n)$ time.

Proof : It suffices to inspect the roots of all binomial trees of the heap. □

- By maintaining a pointer to the root with minimum key, this time can be reduced to $O(1)$. (The pointer can be updated during all operations without increasing the complexity bounds.)

Binomial Heap: Other Operations

Lemma 108

The minimum element can be deleted from a binomial heap with a total of n nodes in $O(\log n)$ time.

Proof : We find the minimum among the roots of the binomial trees. By removing this root we split one binomial tree into a sequence of subtrees which in turn are binomial trees and, thus, form a binomial heap. Now we merge this new binomial heap with the rest of the original binomial heap. All these steps run in $O(\log n)$ time. □

Lemma 109

An element can be deleted from from a binomial heap with a total of n nodes in $O(\log n)$ time.

Proof : We first decrease the key of the element to a value smaller than the minimum key contained in the heap, thus causing it to move upwards to a root, and then delete that root. □

Binomial Heap: Other Operations

Lemma 110

The key of a known element of a binomial heap with a total of n nodes can be decreased in $O(\log n)$ time.

Proof : After decreasing the key we may need to (repeatedly) exchange the corresponding node with its parent node if the min-heap property is violated. Since any binomial tree of the heap has height at most $\log n$, the claim follows. □

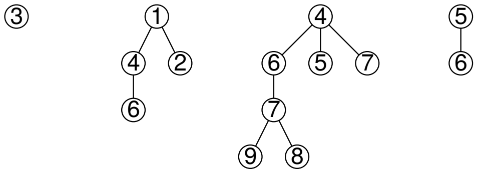
- Note: With the exception of the $O(1)$ bound on the amortized time needed for one insert, all other time bounds are worst-case bounds!

Fibonacci Heaps: Basics

- Designed by Fredman and Tarjan in 1986, in an attempt to improve Dijkstra's shortest-path algorithm from $O((|E| + |V|) \log |V|)$ to $O(|E| + |V| \log |V|)$.
- The name is derived from the fact that the Fibonacci numbers show up in the complexity analysis of its operations.
- Similar to binomial heaps, but less rigid: Fibonacci heaps *lazily* defer all clean-up work after an Insert till the next DeleteMin.

Fibonacci Heap

- Collection of min heaps.
- Maintains pointer to element with minimum key.
- Some nodes are "marked". (Used to keep trees reasonably flat.)



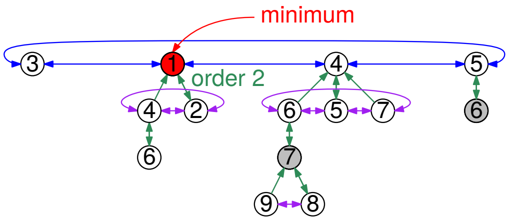
Fibonacci Heaps: Representation

Heap representation:

- Maintain root nodes in doubly-linked circular list.
- Store pointer to root node with minimum key.

Node representation: Every node stores:

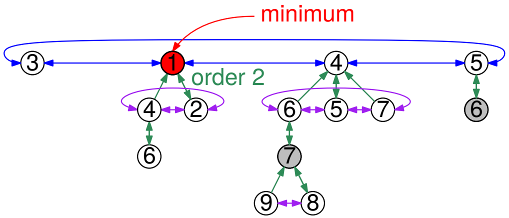
- A pointer to its parent.
- A pointer to one of its children.
- The number of its children (“order”, “rank”).
- Pointers to its left and right siblings.
- A binary flag that indicates whether the node is marked (indicated by gray shading).



Fibonacci Heaps: Marked Nodes

- Marking of nodes:

  Unmarked: The node has had no child cut.
  Marked: The node has had one child cut.
- Basic idea: When a child is cut from a marked parent node, then the parent node (together with its entire subtree) is cut, too, and moved to the root list.
- The marking of nodes ensures that Fibonacci heaps keep roughly the structure of binomial heaps after the deletion of nodes, thus ensuring the amortized time bounds.
- A root node is always unmarked.



Fibonacci Heaps: Basic Operations

Insert a new node:

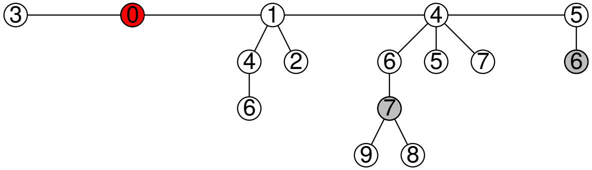
- Create a new node and insert it into the list of root nodes.
- Update pointer to (new) minimum root node.

Link two trees with roots r_1 and r_2:

- If $r_1.key \geq r_2.key$ then make r_1 a child of r_2; otherwise, r_2 becomes a child of r_1.
- Update information on the order of r_2 (or r_1).

Cut a node v (that is not a root node):

- Remove v (and its subtree) from the child list of its parent p and insert it into the root list.
- Update information on the order of p.
- Mark p.

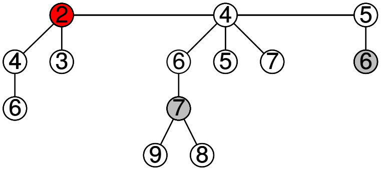


Fibonacci Heaps: DeleteMin

DeleteMin:

- Delete the root node with the current minimum.
- Move its children as new root nodes into the list of root nodes.
- Link trees until no pair of root nodes has the same order.
- Update pointer to minimum root.

First DeleteMin. Second DeleteMin.

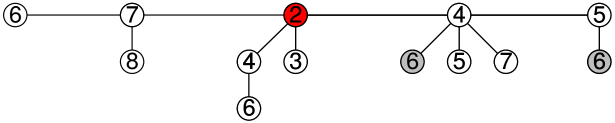


Fibonacci Heaps: DecreaseKey

DecreaseKey:

- If the new key of v is less than the key of the parent p then cut v and move it (with its subtree) to the root list.
- If p is not marked then mark p.
- Else, cut p and move to root list, and apply recursively to its parent.
- Update pointer to minimum root.

DecreaseKey(9,6).



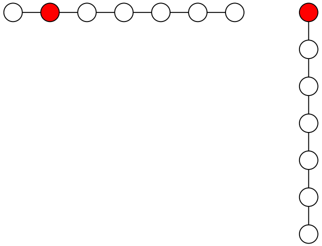
Fibonacci Heaps: Properties

Lemma 111

If only Insert and DeleteMin operations are carried out, then a Fibonacci heap is a binomial heap after every DeleteMin operation.

Sketch of Proof: By induction: Every DeleteMin results in a consolidation phase during which pairs of trees which have root nodes of the same order are linked. □

- If no consolidation occurs (since no DeleteMin operation is carried out) then a Fibonacci heap with n nodes may degenerate to one single tree, or even to an unsorted linked list (of n root nodes) or an "unary" tree of height $n - 1$.



Fibonacci Heaps: Properties

Lemma 112

If a node of a tree in a Fibonacci heap has k children then it is the root of a subtree with at least F_{k+2} nodes.

Corollary 113

Every node of a tree in a Fibonacci heap with a total of n nodes has at most $O(\log n)$ children.

Proof: Let k be the number of children of a node v. By Lem. 112, its subtree has F_{k+2} nodes. Hence,

$$n \geq F_{k+2} \overset{\text{Lem. 5}}{\geq} \phi^k, \quad \text{implying } k \leq \log_\phi n. \qquad \square$$

Fibonacci Heaps vs. Binomial Heaps

Theorem 114

When starting from an initially empty heap, any sequence of a Insert, b DeleteMin and c DecreaseKey operations takes $O(a + b \log n + c)$ worst-case time, where n is the maximum heap size.

- Hence, from a theoretical point of view, a Fibonacci heap is better than a binomial heap when b is smaller than c by a non-constant factor.
- A Fibonacci heap is also better than a binomial heap when frequent merging of heaps is required.
- However, the worst-case time for one DeleteMin or DecreaseKey operation is linear, which makes Fibonacci heaps less suitable for applications which cannot tolerate excessive running times for one individual operation. (E.g., real-time systems.)
- There is some controversy about Fibonacci heaps: While some researchers strongly advocate their use, others report Fibonacci heaps to be slow in practice, due to hidden constants in the O-terms.

Performance Summary of Priority Queues

Performance Summary for Priority Queues with n Elements

Operation	Linked List	Binary Heap	Binomial Heap	Fibonacci Heap
Insert	$O(1)$	$O(\log n)$	$O(1)^{\star}$	$O(1)$
FindMin	$O(n)$	$O(1)$	$O(\log n)^{\star\star\star}$	$O(1)$
DeleteMin	$O(n)$	$O(\log n)$	$O(\log n)$	$O(\log n)^{\star\star}$
DecreaseKey	$O(1)$	$O(\log n)$	$O(\log n)$	$O(1)^{\star\star}$
Merge	$O(1)$	$O(n)$	$O(\log n)$	$O(1)$

*: amortized complexity; worst-case complexity is $O(\log n)$.
**: amortized complexity; worst-case complexity is $O(n)$.
***: can be brought down to $O(1)$ with little extra effort.

- Note: Attempts to get Insert, DeleteMin and DecreaseKey all down to $O(1)$ are doomed to fail. (At least as long as we allow only key comparisons.)

Randomized Data Structures for Searching

Abstract Data Type: Dictionary

Dictionary (Dt.: Wörterbuch)

A *dictionary* is a collection ADT that focuses on data storage and retrieval; i.e., it is a searchable structure.

- Data is a *key-value pair* (KVP), a so-called *item*: (k, v).
- Standard operations:
  - Insert item (k, v) into structure,
  - Retrieve data from structure, i.e., check whether it has an item with a given key k and return the pair (k, v),
  - Delete item from structure.
- In addition, a reassign replaces the value in one of the (k, v) pairs in the structure. Also: Predecessor, successor, join . . .

- Multiple entries with the same key may or may not be allowed. Unless stated otherwise, we assume all keys to be distinct.
- Related terms and synonyms: Key-value database, associative array, map.
- Since the values of the key-value pairs of a dictionary are there only for a piggyback ride, we simply omit the values in the figures and pseudo codes.

Abstract Data Type: Set

Set (Dt.: Menge)

A *set* is a collection ADT that allows to store data items and focuses on efficient membership tests.

- Data items:
    - A data item is a key or key-value pair with trivial value.
    - The order of the data items does not matter (or is undefined),
    - Duplicate data items are not permitted.
- Standard operations:
    - Insert item into structure,
    - Delete item from structure,
    - Test membership, i.e., check whether it has an item with a given key k.
- Core set-theoretic operations for two sets S, T:
    - Union: Compute the union of S and T,
    - Intersection: Compute the intersection of S and T,
    - Difference: Compute the difference of S and T,
    - Subset: Check whether S is a subset of T.

- If duplicate items are allowed: *multiset* or *bag*.

Complexity of Searching

Theorem 115

Comparison-based searching among n elements requires $\Omega(\log n)$ comparisons in the worst case.

Proof : Assume that we want to search for the item that has key k among the items $a_1, a_2, \ldots, a_n$. A decision tree T for solving this problem must contain at least $n + 1$ leaves:

- One leaf for each a_i, if k is the key of a_i.
- One additional leaf for "not found".

Hence, the height of T is at least $\log(n + 1) \in \Omega(\log n)$. □

- We want $O(\log n)$ running time for dictionary operations, where n is the number of items in the dictionary.
- Worst case? Average case? Amortized? Special keys?
- Huge number of results known! We can barely scratch the surface . . .

Balanced Binary Search Trees

Definition 116 (*Height, Dt.: Höhe*)

The *height* of a rooted tree T is the maximum depth of nodes of T, with (by convention) the root of T being at depth 0.

Definition 117 (*Balanced tree, Dt.: balanzierter Baum*)

A binary tree is *(height-)balanced* if it either has no proper subtrees or if

1. it has two proper subtrees and the heights of both subtrees differ by not more than 1, or if
2. it has exactly one proper subtree of height 0,

and if

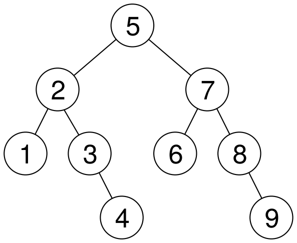
3. all proper subtrees are height-balanced.

Theorem 118

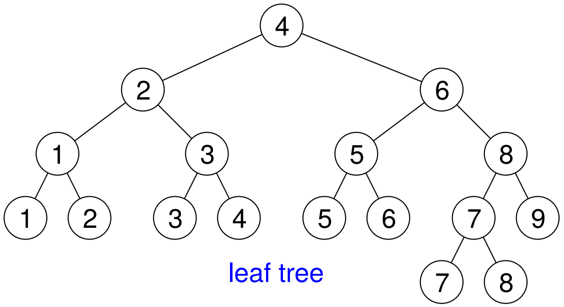
If T is a balanced binary tree with n nodes and height h then $h \in \Theta(\log n)$.

- If T remains balanced after insertions/deletions then it is called *self-balancing*.

Balanced Binary Search Trees: Node Trees and Leaf Trees



node tree



leaf tree

- Node trees became the standard BST tree covered by textbooks because, in most textbooks, the distinction between a value and its key is not made: the key is the value.
- In real applications, the space needed for the actual data associated with a key often is substantially larger than the key itself.
- In such a case the convenience of having only degree-two inner nodes and having all values stored at leaves may well offset the costs of the space consumed by storing additional inner nodes.

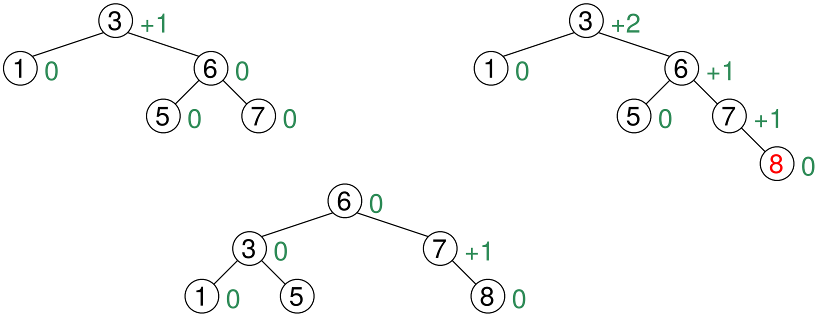
Balanced Binary Search Trees: AVL Trees and Friends

- [Adelson-Vel'skii&Landis (1962)]: First self-balancing binary search tree (BST).
- Rotations to re-balance the tree after insertion or deletion.
- Insertion, searching and deletion all take $O(\log n)$ time in both the average case and the worst case, where n is the number of nodes in the tree.
- AVL insertions require $O(1)$ rotations, while deletions require $O(\log n)$ rotations in the worst case. (But also $O(1)$ on average.)
- Height is at most $\frac{1}{\log \phi} \log n \approx 1.440 \log n \approx 2.077 \ln n$, with $\phi := \frac{1+\sqrt{5}}{2} \approx 1.618$.

- Red-black trees: Have a larger height of at most $2 \log n$, but tend to use fewer rotations. Since AVL trees are more rigidly balanced than red-black trees, they tend to have slower insertion and deletion but faster search.

Balanced Binary Search Trees: AVL Trees and Friends

- Insertion of 8 into sample AVL tree. Rotation to re-balance.



Can we relax the balancing schemes?

Do we need the overhead caused by balancing BSTs? What could be modified?

Randomly Built Binary Search Trees

Random BST

A *randomly built binary search tree* with n nodes is a binary search tree built by inserting n items/keys in random order.

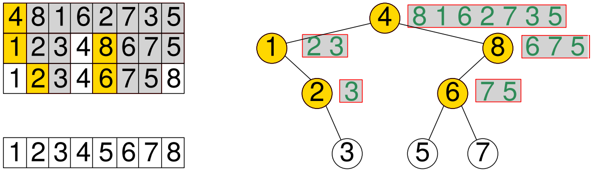
- Of course, this is equivalent to computing a random permutation of the items — where every permutation is equally likely! — and then inserting the items in that order.
- This is different from assuming that every binary search tree is equally likely to occur: Different permutations may result in the same tree!
- It depends on the application whether randomness can be assumed. Otherwise, the resulting tree could be highly skewed.
- What is this good for?
- Well, if you insert 10 numbers in random order then the resulting tree will degenerate to a list with probability $^2/_{10!} \approx 5.511 \cdot 10^{-7}$.
- The more nodes, the less likely the tree is degenerate: It is non-degenerate with high probability.

Randomly Built Binary Search Trees

Lemma 119

The expected time to randomly build a binary search tree with n nodes is $O(n \log n)$.

Sketch of Proof: During the construction of a randomly built BST we perform the same comparisons as a randomized QuickSort, but in a different order. Hence, Theorem 85 is applicable and we also get an $O(n \log n)$ expected-time bound.



□

- Hence, one can also sort in expected $O(n \log n)$ time by constructing a randomly built binary search tree and then applying an inorder traversal.

Randomly Built Binary Search Trees: Node Depth

Lemma 120

The average node depth of a randomly built binary search tree is $O(\log n)$.

Proof : The depth of a node equals the number of comparisons made during the BST construction. Since all permutations of the keys are equally likely, the average node depth d_n is given by

$$d_n = \frac{1}{n}\mathbb{E}\left[\sum_{i=1}^{n}(\#\text{ comparisons for node } i)\right] = \frac{1}{n}O(n\log n) = O(\log n). \qquad \square$$

- Even if the average depth of a node is $\Theta(\log n)$, the height of its tree can still be $\omega(\log n)$.

Theorem 121 (*Reed (2003)*)

A randomly built binary search tree with n nodes has an expected height of $\alpha \ln n$, where $\alpha := 4.311\ldots$ is the unique solution within $[2, \infty)$ of the equation $\alpha \ln(^{2e}/_{\alpha}) = 1$.

- Little is known if insertions *and* deletions are allowed. Deletions destroy randomness [Knott (1975)]; experiments suggest $O(\sqrt{n})$ height.

Randomized Binary Search Trees

[Martínez&Roura (1998)]: Randomized Binary Search Tree

A binary search tree T with n nodes is a *randomized binary search tree* (RBST) if either $n = 0$ or if, for $n > 0$,

1. both its left subtree L and right subtree R are independent randomized binary search trees,
2. $\Pr(L \text{ has } i \text{ nodes}) = \frac{1}{n}$ for all $0 \le i \le n-1$.

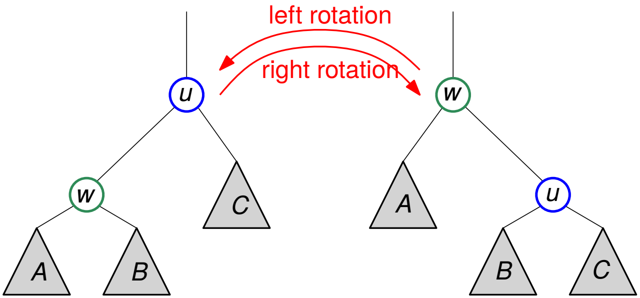
- The randomization implies that every item has the same probability of $1/n$ to be at the root of the tree.
- In an implementation: Pick a random integer k with $0 \le k \le n$, where n is the current number of nodes of T. If $k = n$ then insert at the root of T; otherwise insert recursively into the proper subtree of T.

Theorem 122

The expected height of a randomized binary search tree with n nodes is $O(\log n)$.

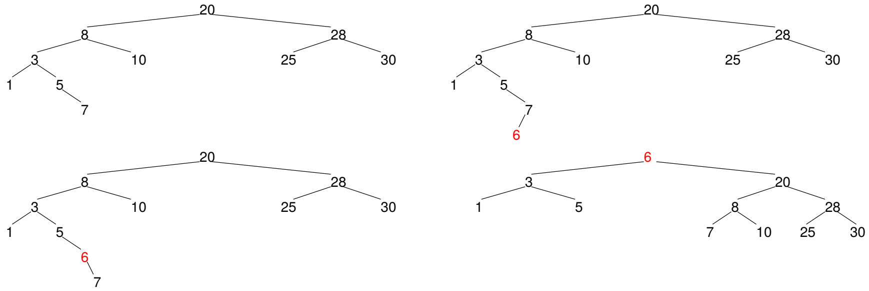
Randomized Binary Search Trees: Rotations

- Simple left and right rotations are carried out in order to maintain the property of being a BST.
- A rotation decreases the depth of one node and increases the depth of another node by one.
- Rotations can be performed in $O(1)$ time because they involve only simple pointer manipulations.



Randomized Binary Search Trees: Sample Insertion at Root

1. Insert new key 6 into sample RBST: As in a standard BST, let key 6 trickle down to appropriate leaf.
2. Move new leaf node that stores 6 upwards, thereby performing left and right rotations:
   right rotation, left rotation, left rotation, right rotation, right rotation.



Randomized Binary Search Trees: Rotations

```
rotateRight(node u, bst T)
{
   node w = u.lft;
   w.parent = u.parent;
   if (u != T.root) {
      if (u.parent.lft == u)     u.parent.lft = w;
      else                       u.parent.rgt = w;
   }
   u.lft = w.rgt;
   if (u.lft != NIL)             u.lft.parent = u;
   u.parent = w;
   w.rgt = u;
   if (u == T.root)              T.root = w;

   return;
}
```

Randomized Binary Search Trees: Rotations

```
rotateLeft(node w, bst T)
{
   node u = w.rgt;
   u.parent = w.parent;
   if (w != T.root) {
      if (w.parent.lft == w)     w.parent.lft = u;
      else                       w.parent.rgt = u;
   }
   w.rgt = u.lft;
   if (w.rgt != nil)             w.rgt.parent = w;
   w.parent = u;
   u.lft = w;
   if (w == T.root)              T.root = u;

   return;
}
```

Randomized Binary Search Trees: Insertion

```
randomizedInsert(key x, bst T)
{
   pick a random number, k, between 0 and T.size, inclusive;
   if (k == T.size) {
      insertAtRoot(x, T);
   }
   else {
      if (x < T.key)    T.lft = randomizedInsert(x, T.lft);
      else              T.rgt = randomizedInsert(x, T.rgt);
   }
}

insertAtRoot(key x, bst T)
{
  use standard BST algorithm to insert x as a leaf in T;

  perform left/right rotations to move the node containing x
          all the way up to the root of T;
}
```

Randomized Binary Search Trees: Deletion

- We make use of a *join* operation for two RBSTs L and R, where all keys in L are assumed to be less than all keys in R:
  - Let n_L be the size of L, and n_R be the size of R.
  - Use root of L as root of the union tree with probability ${}^{n_L}/_{n_L+n_R}$, and recursively join right subtree of L with R.
  - Use root of R as root of the union tree with probability ${}^{n_R}/_{n_L+n_R}$, and recursively join L with left subtree of R.
- Deletion:
  - Search and delete the node that contains the key sought.
  - Use join operation to join the two subtrees of that node.

Lemma 123

Tree is still random after deletion.

Theorem 124

The expected height of a randomized binary search tree with n nodes is $O(\log n)$. Search, insertion, deletion and join all run in $O(\log n)$ expected time.

Randomized Binary Search Trees: Deletion

```
randomizedJoin(bst L, bst R)
{
   pick a random number, k, between 1 and (L.size + R.size);
   if (k <= L.size) {
      T = L;
      T.rgt = randomizedJoin(L.rgt, R);
   }
   else {
      T = R;
      T.lft = randomizedJoin(L, R.lft);
   }
}

delete(key x, bst T)
{
   search node N such that N.key equals x;
   randomizedJoin(N.lft, N.rgt);
   remove(N);
}
```

Treaps

Treap [Vuillemin (1980)]

A *treap* is a binary tree in which every node stores a priority in addition to the key-value pair such that

- it is a binary search tree on the keys,
- it is a max-heap on the priorities, where greater number means higher priority.

- All keys and priorities are assumed to be distinct.
- Rediscovered and used as RBSTs by Aragon&Seidel (1989).

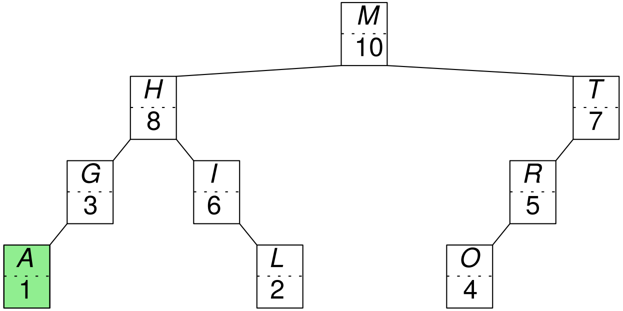
Lemma 125

The structure of a treap is completely determined by the search keys and priorities of its nodes.

Sketch of Proof : We use induction. The base case is the treap with at most one node. Since a treap is a heap, the node with highest priority must be at its root. Since a treap is a BST, all nodes in its left subtree need to have keys less than the key of the root, and all nodes in its right subtree need to have keys greater than the key of the root. Since subtrees are treaps themselves, their structure is completely determined by the inductive hypothesis. □

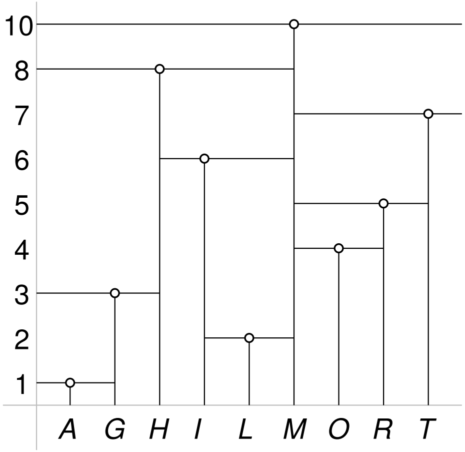
Treaps: Construction

- In the figures we use letters for the search keys and integers for the priorities.
- The proof of Lemma 125 suggests a way to construct a treap for a given set of key-(value-)priority triples:



Treaps: Alternate Characterization

- Alternate characterization of treaps, with proof by induction:
  1. Sort nodes by priority.
  2. Insert one node at a time into BST according to key.
- Yet another geometric characterization:
  1. Regard key-priority pairs as coordinates in $\mathbb{R}^2$.
  2. Recursively split (portions of) the plane by inserting T-shaped boundaries.



Treaps: Operations

Search:

- Since a treap is a BST, we can apply the algorithm for searching in a BST.

Insertion:

- We use the algorithm for insertion into a BST, thus creating a node z.
- In order to repair the heap structure, we use rotations to “bubble” z upwards as long as z has a greater priority than its parent.

Deletion:

- Search the node z sought.
- Use rotations to push z downwards until it becomes a leaf, thereby moving its higher-priority child upwards. (Inverse rotations as for insertion!)

Split: Split treap T into two treaps T_1, T_2 such that all keys of T_1 are less than some given key x and all keys of T_2 are greater than x.

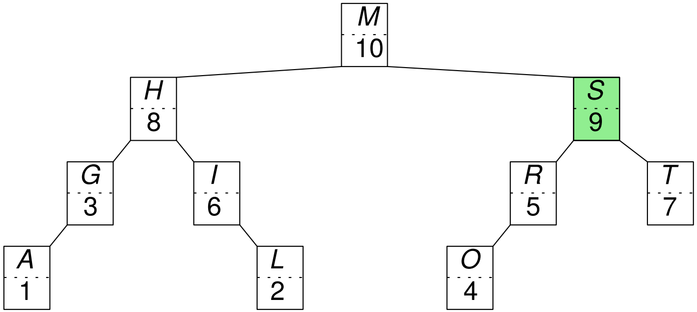
- Insert a dummy node with key x and priority $+\infty$ into T.
- This node will become the root of the new treap, and its subtrees form the two treaps T_1, T_2 sought.

Lemma 126

The cost of each of these operations is proportional to the height of the treap.

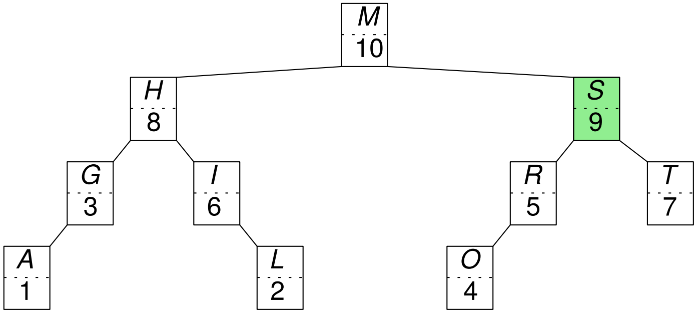
Treaps: Sample Insertion

- Insertion of item with key *S* and priority 9: Create new leaf node at appropriate place. Left rotation to bubble up. Right rotation to bubble up.



Treaps: Sample Deletion

- Deletion of node with key S: Left rotation to push node down. Right rotation to push down. Deletion of node.



Treaps: Operations

```
bubbleUp(node z, treap T)
{
   while ((z.parent != NIL)  &&  (z.parent.p > z.p)) {
      node u = z.parent;
      if (z.parent.rgt == z)     rotateLeft(z.parent, T);
      else                       rotateRight(z.parent, T);
      z = u;
   }
   if (z.parent == NIL)          T.root = z;

   return;
}
```

Treaps: Randomization

Randomized Treap

A *randomized treap* is a treap in which the priorities are independently and uniformly distributed continuous random variables.

- Typically, the term “treap” has come to mean almost exclusively “randomized treap”, and it is common to drop the word “randomized”.
- When inserting a new key-value pair we generate a random real number between, e.g., 0 and 1, and use that number as the priority of the new node.
- By using reals as priorities we ensure that the probability of two nodes having equal priority is zero. In practice, choosing a random integer from a large range or a random floating-point number is good enough.
- Since the priorities are independent, each node is equally likely to have the largest priority and, thus, to be at the root of the treap.
- Hence, a *(randomized) treap is a randomized binary search tree!* Lemma 126 implies the following main result. (A formal proof is very similar to RBSTs.)

Theorem 127

The expected height of a treap with n nodes is $O(\log n)$. Search, insertion, deletion and split all run in $O(\log n)$ expected time. The expected number of rotations done during an insertion/deletion is only $O(1)$.

Sorted Linked List

Pros

- Truly simple dynamic data structure that is easy to implement.
- No need for an a-priory estimate of the number of elements to be stored.
- Easy to insert or delete in $O(1)$ time if position is known.

Cons

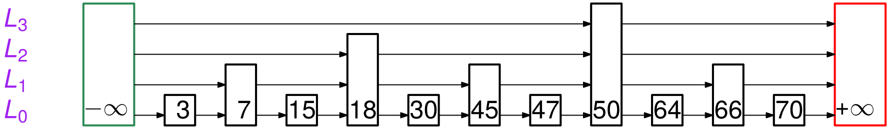
- Difficult to get to the middle of the list; binary search does not work.
- Search in $o(n)$ expected time is difficult even if all elements are distinct.

- Searching a sorted listed requires $\Omega(n)$ time if multiple elements may have the same key.

- Goal: Combine the appealing simplicity of sorted lists with a good expected-time behavior!

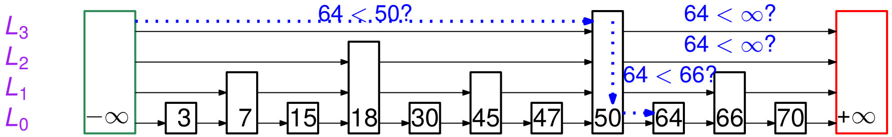
Perfect Skip Lists

- Idea: Add a second list L_1 containing only every second item. Then we need at most $\lceil \frac{1}{2} n \rceil$ comparisons on L_1 and, with proper links into the first list L_0, one additional comparison on L_0 to carry out a search.
- If k nested lists are used: At most $\lceil \frac{1}{2^{k-1}} n \rceil$ comparisons on the k-th list L_{k-1}, plus one additional comparison in each of the lists $L_0, L_1, \ldots, L_{k-2}$.
- This will get us $O(\log n)$ search time for $k := O(\log n)$.
- Header and sentinel nodes are in every level.
- Nodes are of variable size: Contain between 1 and $O(\log n)$ pointers.
- The number of pointers does not change after an insertion; can use array to store the pointers.



Perfect Skip Lists: Search

- To search for an item given a query key, we start on the list at the top level.
- In the current list we move towards the sentinel until the key of the next item will be greater than the query key.
- Then we go down and repeat the procedure, until we are in the bottom list L_0.
- In the bottom list L_0 we either find the item queried, or no such item exists.
- When searching for k:
  If $k = next.k$: done!
  If $k > next.k$: go right. Stop at sentinel.
  If $k < next.k$: go down one level from L_i to L_{i-1}. Stop at L_0.
- $O(\log n)$ levels, and will visit at most 2 nodes per level: $O(\log n)$ search time.



Perfect Skip Lists: Search

- The following sample code for a search in a skip list assumes the existence of a sentinel key that is guaranteed to be greater than any search key.

```
searchSkipList(key x, skiplist T)
{
   Node u = T.header;
   int  h = T.height;
   while (h >= 0) {
      while (u.next[h].key < x) /* assumes sentinel */
         u = u.next[h];
      --h;
   }

   return u;
}
```

Skip Lists

- Maintaining perfect skip lists after insertions and deletions may require re-arranging the entire structure . . .
- Goal: Design a hierarchical structure of singly-linked lists such that we can expect about $1/2$ the items at the next higher level.
- [Pugh (1989)]: Probabilistic skip lists refine the idea of using a linked hierarchy of sublists by dropping the constraint that lists jump a number of items that equals a power of two.
- Skip lists achieve expected $O(\log n)$ complexity for search, insert and delete operations.
- Skip lists are "better trees", but remain about as easy to implement as standard sorted linked lists.

  "Skip lists are a probabilistic data structure that seem likely to supplant balanced trees as the implementation method of choice for many applications. Skip list algorithms have the same asymptotic expected time bounds as balanced trees and are simpler, faster and use less space." *[Pugh (1989)]*

- Actual timings for the same sequence of operations may vary depending on the random choices made by the data structure.

Skip Lists: Insertion and Removal

- Allow for some imbalance. Still, the expected behavior (over the random choices) shall remain the same as with perfect skip lists.
- Insertion:
  - Insert item into full list L_0, i.e., at the lowest level 0.
  - Promote it to the next higher level with (independent) probability p.
- Common choices for p are $1/2$ and $1/4$.
- Choice of p allows a trade-off between space complexity and query speed.
- We focus on $p = 1/2$: Then the highest level of a newly inserted item can be determined by repeatedly flipping a coin until the coin comes up heads.
- Level structure of a skip list is independent of the keys inserted. The expectation is over the random coin flips. Hence, there are no “bad” key sequences that might cause a skip list to degenerate.
- Deletion: Search and then remove item from structure.
- With some very small probability, the skip list will just be a linked list, or the skip list will have every node at every level.
- Note: Parallel insertions or deletions are relatively easy to support!

Skip Lists: Analysis

- The height of a skip list is the number of its levels, with the bottom-most list L_0 at level 0.

Lemma 128

The expected number of times a fair coin is tossed up to and including the first time the coin comes up heads is 2.

Proof: Let T denote this random variable and define an indicator random variable I_i as $I_i := 1$ if the coin ends up being tossed i or more times, and $I_i := 0$ otherwise. We have

$$\mathbb{E}(I_i) = \Pr(I_i = 1) = \frac{1}{2^{i-1}} \qquad \text{and} \qquad T = \sum_{i=1}^{\infty} I_i.$$

This gives

$$\mathbb{E}(T) = \mathbb{E}(\sum_{i=1}^{\infty} I_i) = \sum_{i=1}^{\infty} \mathbb{E}(I_i) = \sum_{i=1}^{\infty} \frac{1}{2^{i-1}} = \sum_{i=0}^{\infty} \frac{1}{2^i} = 2. \qquad \square$$

- Hence, the expected number of levels for a newly inserted item is 2!

Skip Lists: Analysis

Lemma 129

Suppose that we use constant-size nodes, with one node per level if an item is stored in that level. Then the expected number of nodes in a skip list storing n items is $2n$ if we disregard header and sentinel nodes.

Proof : The probability of an item to be included in list L_i is $^1/_{2^i}$. Therefore the expected number of nodes in L_i is $^n/_{2^i}$ and we get

$$\sum_{i=0}^{\infty} \frac{n}{2^i} = n \sum_{i=0}^{\infty} \frac{1}{2^i} = 2n$$

as the total expected number of nodes. □

- Hence, linear storage can be expected to suffice for storing a skip list.

Skip Lists: Analysis

Lemma 130

The expected height of a skip list storing n items is at most $\log n + 2$.

Lemma 131

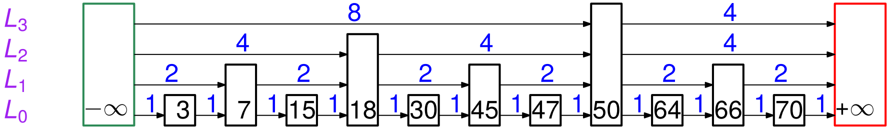
The expected length of a search path in a skip list storing n items is $2\log n + 2$.

Theorem 132

A skip list storing n items has expected size $O(n)$ and supports search, insertion and deletion in expected time $O(\log n)$.

Skip Lists: Indexable Lists

- We can count the number of edges in a search path, in order to gain access to the *j*-th item stored in the skip list:
  - length of edge in L_0 is 1,
  - length of edge in L_i is the sum of the lengths of the edges in L_{i-1} below it.
- To get to the *j*-th node we
  - go right if the sum of the edge lengths so far plus the length of the next edge is less than *j*,
  - go down otherwise.
- This makes it easy to get the *j*-th item in the sorted list in $O(\log n)$ time, and to set/modify its value. Within the limits imposed by the fact the sequence has to remain sorted, we can even modify its key.
- Faster get/set than linked list; faster add/delete than array-based list.
- Sample application: Computation of so-called *running median* on a stream of data.



Skip Lists: Implementational Issues

Insertion: To insert item k with key x we

- pick a height h for k by flipping coins,
- create a node for k with space for h next pointers,
- follow the search path for x downwards: if $i \leq h$ then we insert k into L_i by straightforward splitting and splicing.

Deletion: To delete item k with key x we

- follow the search path for x downwards: when the node containing k is immediately to the right then we splice out that node.

Skip Lists: Implementational Issues

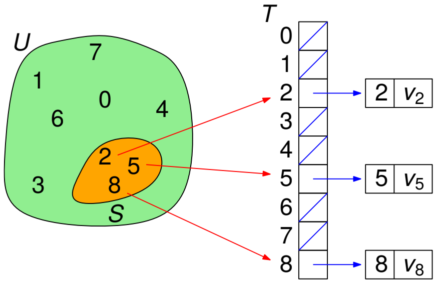
```
insertProbabilisticSkipList(key x, skiplist T)
{
   Node u  = T.header;
   int  h  = T.height;
   int  hx = result of coin flips;
   Node v  = CreateNode(x, hx);
   while (h >= 0) {
      while (u.next[h].key < x) /* assumes sentinel */
         u = u.next[h];
      if (h <= hx) {
         v.next[h] = u.next[h];
         u.next[h] = v;
      }
      --h;
   }
   ++T.counter_of_nodes;
   return v;
}
```

Skip Lists: Implementational Issues

```
deleteProbabilisticSkipList(key x, skiplist T)
{
   Node u   = T.header;
   int  h   = T.height;
   boolean removed = false;
   Node v   = CreateNode(x, hx);
   while (h >= 0) {
      while (u.next[h].key < x) /* assumes sentinel */
         u = u.next[h];
      if (u.next[h].key == x) {
         removed = true;
         u.prev[h].next[h] = u.next[h]; /* can avoid prev */
      }
      --h;
   }
   if (removed) --T.counter_of_nodes;
   return removed;
}
```

Direct Addressing

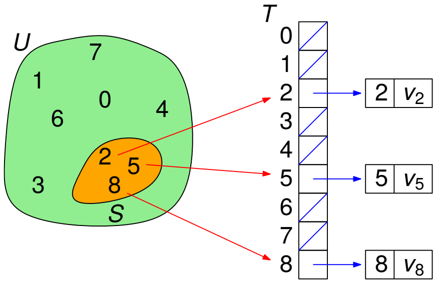
- Can we realize a data structure for maintaining dynamic sets that supports insert, retrieve and delete operations in $O(1)$ time?
- Suppose that every key-value pair has a key drawn from the universe $U := \{0, 1, \ldots, n-1\}$, for some $n \in \mathbb{N}$. (I.e., $U = \mathbb{Z}_n$.)
- In order to represent a dynamic set S of KVPs we could use a *direct-address table* of size n, denoted by $T[0, 1, \ldots, n-1]$:



- If S contains the key-value pair (k, v) then we store a pointer to v in $T[k]$, and *NIL* otherwise.

Direct Addressing

- Direct Addressing: The standard dictionary operations insert, retrieve and delete are trivial to implement, provided that all key-value pairs have distinct keys.
- Each operation runs in $O(1)$ time.
- Obvious drawbacks:
  - If $|U|$ is large then it may be impractical or even impossible to store a table of size $|U|$.
  - If $|S| \ll |U|$, then allocating a table of size $|U|$ is a waste of memory.



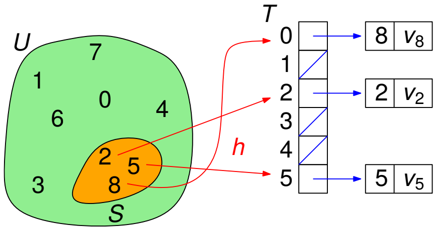
- Can we trade $O(1)$ worst-case complexity for $O(1)$ average-case complexity and reduce the memory requirement to $\Theta(|S|)$?

Basics of Hashing

Hash function, Dt.: Streuwertfunktion

A *hash function*, $h\colon U \to \mathbb{Z}_m$, maps a key k of the universe U to the *slot* (aka *bucket*) $h(k)$ of the *hash table* $T[0, 1, \dots, m-1]$, for $m \in \mathbb{N}$.

- We say that k *hashes* to $h(k)$, and $h(k)$ is the *hash value* of k.
- Pick appropriate m and use hash function that can be evaluated in constant time.

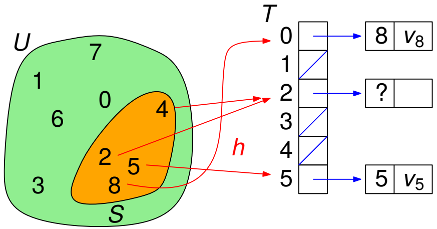


Basics of Hashing

Hashing

A *hash function*, $h: U \to \mathbb{Z}_m$, maps a key k of the universe U to the *slot* (aka *bucket*) $h(k)$ of the *hash table* $T[0, 1, \dots, m-1]$, for $m \in \mathbb{N}$.

- If $m < |S|$ then the pigeonhole principle implies that at least two keys will hash to the same slot, for any hash function h. Could happen also for $m \geq |S|$!
- Such a situation is called a *collision*, which we need to resolve.

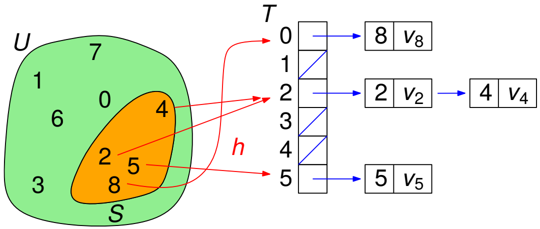


Standard methods for resolving collisions:

- Chaining: Use a list for $T[h(k)]$.
- Open addressing: Allow alternate slots instead of $h(k)$. Lazy deletion; insertion is $\Theta(1)$ only on average.

Resolving Collisions: Separate Chaining

- Chaining: Rather than letting $h(k)$ point to a single memory cell that stores v, we let it point to a list which contains all KVPs whose keys hash to the same slot.
- Dt.: Hashing mit Verkettung.



Resolving Collisions: Separate Chaining

- Chaining: Rather than letting $h(k)$ point to a single memory cell that stores v, we let it point to a list which contains all KVPs whose keys hash to the same slot.
- Then insertion maintains its $O(1)$ worst-case complexity (if we may assume that the KVP to be inserted is not yet present in the hash table).
- The complexity of retrieving a KVP depends on the (maximum) length of a list.
- Worst-case complexity of retrieval: $\Theta(n)$ if n KVPs have been stored in the table in a single list.
- An actual deletion of a KVP (upon its prior location) can be done in $O(1)$ time (if doubly-linked lists are used).
- Denote the length of the list referenced by $T[i]$ by n_i. We have

$$n_0 + n_1 + \cdots + n_{m-1} = n.$$

- Can we say anything on $\mathbb{E}(n_i)$ and, thus, on the expected complexity of a search?

Resolving Collisions: Separate Chaining

Definition 133 (*Load factor*)

Let a hash table T store n KVPs in a total of m slots. The *load factor* α of T is defined as

$$\alpha := \frac{n}{m}.$$

Uniform hashing

A key k is equally likely to hash into any of the m slots, independently of where any other key has hashed to.

- Hence, with uniform hashing we have

$$\Pr\left(h(k) = i\right) = \frac{1}{m} \qquad \text{for all } i \in \{0, 1, \dots, m-1\} \text{ and all } k \in U,$$

and

$$\mathbb{E}(n_i) = \sum_{j=0}^{n-1} 1 \cdot \Pr\left(h(k_j) = i\right) = \sum_{j=0}^{n-1} \frac{1}{m} = \frac{n}{m} = \alpha.$$

Resolving Collisions: Separate Chaining

Lemma 134

If uniform hashing is used and collisions are resolved by chaining then an unsuccessful search runs in expected time $\Theta(1+\alpha)$.

Proof: Any new key k is equally likely to hash to any of the m slots. The expected time to search unsuccessfully for k in the list of $T[h(k)]$ is the time needed to search the list to its end, which has expected length α. □

- The situation for a successful search is slightly different because each list is not equally likely to be searched: If all stored KVPs are assumed to be equally likely to be retrieved then the probability that a list is searched is proportional to the number of KVPs which it contains.
- Still, one can prove that a successful search can be expected to involve $1+\frac{\alpha}{2}-\frac{\alpha}{2n}$ items.

Theorem 135

If uniform hashing is used and collisions are resolved by chaining then any search runs in expected time $\Theta(1+\alpha)$.

- Obvious goal: Ensure that $\alpha = O(1)$. E.g., ensure $\alpha \leq 2$.

Re-Hashing

- Assume that repeated insertions caused the load factor α to get too big.
- Then it is common to double m, thus getting a new $m^\star \approx 2m$ as new size of the hash table, implying a new load factor $\alpha^\star \approx \frac{1}{2}\alpha$:
  - Find a new hash function $h^\star : U \to \mathbb{Z}_{m^\star}$.
  - Re-hash: Insert each KVP from old hash table into new hash table.
- Same as for dynamic arrays, this adds $O(m^\star + n)$ time to one particular insertion, but happens rarely: It adds $O(1)$ amortized time to insertion.
- Re-hashing ensures that $\alpha \in O(1)$.

Theorem 136

If uniform hashing — with re-hashing as outlined above — is used and collisions are resolved by chaining then insertion, retrieval and deletion run in expected amortized time $O(1)$.

- But worst-case time is $\Theta(n)$ for a hash table with n KVPs!

Choosing a “Good” Hash Function

- The analysis of hashing based on separate chaining relies on the assumption that the hash function satisfies the condition of uniform hashing.
- If the keys are random real numbers distributed independently and uniformly in the range $[0, 1[$ then

  $$h(k) := \lfloor k \cdot m \rfloor$$

  satisfies the condition of uniform hashing.
- However, in general this assumption is difficult to support in practice:
  - We will rarely know the probability distribution from which the keys are drawn.
  - Worse, the keys might not be drawn independently.
- Hence, heuristics are employed that tend to work well in practice.

Choosing a “Good” Hash Function: Modular Hashing

Modular hashing

$h(k) := k \bmod m$.

- Aka: Division method.
- We need to choose m carefully!
- If m is a power of 2, say $m := 2^p$, then $h(k)$ would amount to the p lowest-order bits of k.
- This is a very poor choice for h unless we were guaranteed that all low-order p-bit patterns of the keys are equally likely.
- Similarly, if $m := 2^p - 1$ and k is a character string interpreted in radix 2^p, then permuting the characters of k would not result in a different hash value: We have

$$a \cdot (2^p)^i + b \cdot (2^p)^j \equiv_m a \cdot (1)^i + b \cdot (1)^j = a + b \equiv_m a \cdot (2^p)^j + b \cdot (2^p)^i.$$

- Prime numbers not too close to a power of 2 (or power of 10) work well in practice as a choice for m.

Choosing a “Good” Hash Function: Multiplication Method

Multiplication method

Let $x \in \mathbb{R}$ with $0 < x < 1$. Then

$$h(k) := \lfloor m \cdot (x \cdot k \bmod 1) \rfloor,$$

where $x \cdot k \bmod 1 := x \cdot k - \lfloor x \cdot k \rfloor$, i.e., $x \cdot k \bmod 1$ is the fractional part of $x \cdot k$.

- This is a generalization of modular hashing: If $x := \frac{1}{m}$ then

$$h(k) = \left\lfloor m \left(\left(\frac{1}{m} \cdot k \right) \bmod 1 \right) \right\rfloor = \left\lfloor m \frac{(k \bmod m)}{m} \right\rfloor = k \bmod m.$$

- [Knuth, TAoCP Vol. 3 (1973)]: Supposedly $x := \frac{\sqrt{5}-1}{2}$ works well (“Fibonacci hash”).
- The multiplication method tends to yield hashes with decent “randomness” for the same reason why linear congruential generators work.
- The choice of m is not so critical, and there seems to be some disagreement on what is best.

Universal Hashing

- For some fixed hash function, a malicious adversary can always choose n keys which all hash to the same slot, yielding an average retrieval time of $\Theta(n)$.

Universal hashing, Dt.: Universelles Hashing

The hash function is chosen randomly (from a diligently designed class of hash functions) in a way which is independent of the keys that will be stored.

- Pro: As for randomized quicksort, randomization guarantees that no sequence of inputs/operations will always result in a worst-case performance.
- Con: Universal hashing may (and, likely, will) behave differently for each execution, even when supplied with the same sequence of inputs/operations.

Definition 137 (*Universal collection of hash functions*)

Let $m \in \mathbb{N}$ and $\mathcal{H}$ be a finite collection of hash functions that map a universe U of keys to $\{0, 1, \ldots, m-1\}$. This collection of hash functions is *universal* if

$$|\{h \in \mathcal{H} : h(k) = h(i)\}| \leq \frac{|\mathcal{H}|}{m}$$

for each pair of distinct keys $k, i \in U$.

Universal Hashing

Lemma 138

Let $m \in \mathbb{N}$ and $\mathcal{H}$ be a universal collection of hash functions. Consider a pair of distinct keys $k, i \in U$ and pick a hash function h randomly from $\mathcal{H}$. Then

$$\Pr(h(k) = h(i)) \leq \frac{1}{m}.$$

Proof: There are at most $\frac{|\mathcal{H}|}{m}$ hash functions with $h(k) = h(i)$, out of a total of $|\mathcal{H}|$ hash functions. □

- Hence, the probability of a collision is exactly the same as when choosing $h(k)$ and $h(i)$ randomly and independently from $\mathbb{Z}_m$.
- We will now analyze the expected complexity of universal hashing that uses separate chaining to resolve collisions.
- Note: The expectations will be over the choice of the hash function! No assumption is made about the distribution of the keys.

Universal Hashing

Theorem 139

Let $m \in \mathbb{N}$ and $\mathcal{H}$ be a universal collection of hash functions. Pick a hash function h randomly from $\mathcal{H}$ and suppose that it has been used to hash n keys into a hash table T of size m, with separate chaining used to resolve collisions.
If the key k is not in T then

$$\mathbb{E}(n_{h(k)}) \leq \alpha.$$

If the key k is in T then

$$\mathbb{E}(n_{h(k)}) \leq 1 + \alpha.$$

Universal Hashing

Theorem 140

Let T be an initially empty hash table with m slots, with separate chaining used to resolve collisions. If universal hashing is used then any sequence of N insert, retrieve and delete operations that contains $O(m)$ insert operations runs in $\Theta(N)$ expected time.

Proof : Since we have $O(m)$ inserts among a total of N operations, we get $n = O(m)$ and, thus, $\alpha = O(1)$. Then Theorem 139 tells us that one search runs in expected time $O(1)$. Same for one insert or one delete (once position is known).
By linearity of expectation, the expected time of the entire sequence is $O(N)$ and, thus, also $\Theta(N)$. □

- What remains to be done is to design a universal collection of hash functions . . .

Universal Hashing

- Let $p \in \mathbb{P}$ be a prime number large enough such that $U \subseteq \mathbb{Z}_p$ and such that $p > m$.

Definition 141

For $a \in \mathbb{Z}_p^+$ and $b \in \mathbb{Z}_p$, we define the hash function $h_{a,b,p,m} \colon \mathbb{Z}_p \to \mathbb{Z}_m$ as follows:

$$h_{a,b,p,m}(k) := ((a \cdot k + b) \bmod p) \bmod m.$$

Then

$$\mathcal{H}_{p,m} := \{h_{a,b,p,m} : a \in \mathbb{Z}_p^+, b \in \mathbb{Z}_p\}.$$

- We have $|\mathcal{H}_{p,m}| = (p-1) \cdot p$.

Theorem 142 (*Carter&Wegman (1979)*)

The class $\mathcal{H}_{p,m}$ is a universal collection of hash functions.

Choosing a “Good” Hash Function: Strings as Keys

- Most hash functions assume that all keys belong to $\mathbb{N}_0$.
- Standard way to map a character string s to an integer: Interpret the string as an integer expressed in a suitable radix notation.
- E.g., since $p \sim 112$, $t \sim 116$ and $r \sim 114$ in the 7-bit ASCII code, we can regard the string $s := \texttt{ptr}$ as the triple $(112, 116, 114)$.
- Expressed as a radix-R integer, with radix $R := 128$ (or radix $R := 256$), we get the mapping

$$f(s) = 128^2 \cdot 112 + 128 \cdot 116 + 114 = 1849970.$$

- Now use $f(s)$ as argument for the hash function.
- Note: $f(s)$ can be truly huge! Hence, apply modulo computations early and do not compute the powers of the radix explicitly.

$$f(s) = 128 \cdot (128 \cdot 112 + 116) + 114 = 1849970.$$

Choosing a “Good” Hash Function: Strings as Keys

```
int StringModularHash(string S,      // string in ASCII
                      int R,         // radix
                      int M)         // modulus
{
   N = S.length - 1;
   int h = S[N];                     // modular hash of S
   for (i = N-1;  i >= 0;  --i) {
      h *= R;
      h += S[i];
      h  = h mod M;
   }

   return h;
}
```

Perfect Hashing

- *Static set of keys*: Assume that the set of keys does not change once stored in the hash table. (E.g., consider the set of reserved words for a programming language, or the names of streets of a map uploaded to a navigation system.)
- Goal: Improve the excellent average-case performance of (universal) hashing to an excellent worst-case performance.

Perfect Hashing [Fredman&Komlós&Szemerédi (1984)]

Perfect hashing is a two-level hash scheme, with universal hashing at each level. The secondary hashing is injective, thus guaranteeing $\Theta(1)$ search time for a set of keys known a priori.

- Let $p \in \mathbb{P}$ be a prime number large enough such that $U \subseteq \mathbb{Z}_p$ and $p > m$.
- We hash n keys of U into m slots of T using universal hashing with open chaining. This primary hash function belongs to $\mathcal{H}_{p,m}$ and is of the form

$$h_{a,b,p,m}(k) := ((a \cdot k + b) \bmod p) \bmod m,$$

with $a \in \mathbb{Z}_p^+$ and $b \in \mathbb{Z}_p$.

Perfect Hashing

Lemma 143

If we store n keys in a hash table of size $m := n^2$ by using a hash function randomly chosen from a universal collection of hash functions, then we get collisions with a probability of less than $\frac{1}{2}$.

- Hence, after trying a few randomly chosen hash functions, we will have found a hash function that does not yield collisions with very high probability: The probability that we have found a hash function without collisions after trying i hash functions is at least $1 - \frac{1}{2^i}$.
- Let Y be the random variable that represents the number of hash functions that need to be tried until no collision occurs. We have

$$\mathbb{E}(Y) = \sum_{i=1}^{\infty} 1 \cdot \Pr(Y \geq i) \leq \sum_{i=1}^{\infty} \frac{1}{2^{i-1}} = \sum_{i=0}^{\infty} \frac{1}{2^i} = 2.$$

  Hence, we can expect that two random tries of hash functions suffice.
- Still, it is obvious that a hash table of size n^2 is excessively large . . ..

Perfect Hashing

- Still, it is obvious that a hash table of size n^2 is excessively large.
- For the primary hash table we use $m := n$, resulting in $O(n)$ memory being consumed by the primary hash table.
- We apply this idea in a second round of hashing: The n_j keys hashed to a slot j of T are re-hashed by a secondary hash function into a secondary hash table S_j of size $m_j := n_j^2$, using a hash function h_j chosen from $\mathcal{H}_{p,m_j}$.
- Of course, besides ensuring that no collisions occur in S_j, the overall space complexity shall remain linear.

Lemma 144

We store n keys in the primary hash table T of size $m := n$, using a hash function randomly chosen from a universal collection of hash functions. Let n_j be the number of keys hashed into slot j, and let $m_j := n_j^2$ be the size of the secondary hash table S_j. Then the expected amount of memory consumed by all secondary hash tables is less than $2n$.

Perfect Hashing

Theorem 145

Perfect hashing allows to store a fixed set of n keys in expected $O(n)$ time and space in a two-level hash table such that search queries can be answered in worst-case $O(1)$ time.

- *Dynamic perfect hashing:* The hash function is updated whenever the set of keys changes. Allowing updates makes the situation quite messy, though . . .
- So, can we get something similarly good as perfect hashing but still allow updates?

Cuckoo Hashing

Cuckoo Hashing [Pagh&Rodler (2001)]

Cuckoo hashing is a variant of open addressing that uses two hash functions h_1, h_2 such that any key k is always either at slot $h_1(k)$ or at $h_2(k)$.

- Hence, search and delete operations are trivial and run in $O(1)$ worst-case time.
- The two hash functions may address the same hash table or two different tables.

Theorem 146

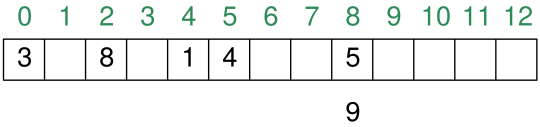
Cuckoo hashing guarantees worst-case $O(1)$ search and delete times. If the load factor is kept less than $\frac{1}{2}$ then an insert runs in expected $O(1)$ time.

- The bound on the expected time of insertion is rather tricky to prove. We sketch only how insertions work.
- Experiments suggest that cuckoo hashing is much faster than chaining for small hash tables, and slightly worse than perfect hashing. But it is dynamic!
- Variation: Use three or more hash functions to allow to increase the load factor.

Cuckoo Hashing: Insertion

- If $T[h_1(k)]$ is empty, then insert k at $T[h_1(k)]$.
- Else, if $T[h_2(k)]$ is empty then insert at $T[h_2(k)]$.
- If both $T[h_1(k)]$ and $T[h_2(k)]$ are full then
  1. "kick the key k_1 stored at $T[h_1(k)]$ out of the nest",
  2. store k at $T[h_1(k)]$,
  3. store k_1 at $T[h_2(k_1)]$; if $T[h_2(k_1)]$ is occupied by k_2 then "kick k_2 out of the nest", alternating between h_1 and h_2, etc.
- To prevent a loop (or large number of iterations) we break after some number i (that is logarithmic in m) of iterations and re-build the hash table with larger m.

$$h_1(8) = 2, h_2(8) = 8$$
$$h_1(4) = 0, h_2(4) = 5$$
$$h_1(1) = 4, h_2(1) = 5$$
$$h_1(9) = 0, h_2(9) = 8$$
$$h_1(5) = 0, h_2(5) = 8$$
$$h_1(3) = 0, h_2(3) = 4$$



0	1	2	3	4	5	6	7	8	9	10	11	12
3		8		1	4			5				
								9				

Data Structures for Geometric Queries

Introduction to Geometric Searching

Point-Inclusion Query: In which “object” or “cell” (of, e.g., a map) does a query point lie?

Range Searching:

- **Report Query**: Which points are within a query object (rectangle, circle)?
- **Count Query:** Only the number of points within an object matters.

- Another way to distinguish geometric searching queries:

Single-Shot Query: Only one query per data set.

Repetitive-Mode Query: Many queries per data set; preprocessing may make sense.

- The complexity of a query is determined relative to four cost measures:
  - query time,
  - preprocessing time,
  - memory consumption,
  - update time (in the case of dynamic data sets).

Range Searching: Report Query

Problem: RANGESEARCHREPORT

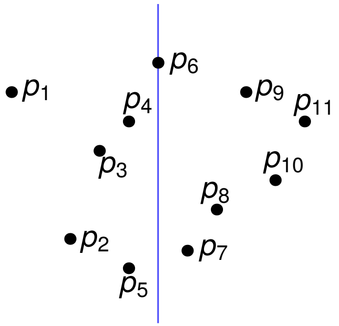
Input: A set S of n points in $\mathbb{R}^k$ and a query (hyper-)rectangle $\mathcal{R}$.

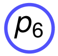
Report: Those m points of S which are within $\mathcal{R}$.

- General position assumed: No two points of S have the same coordinate value in any dimension. (There are workarounds ...)
- Case $k = 1$: Then the rectangle $\mathcal{R}$ is an interval.
  - As preprocessing we sort the points and store them in an array. This needs $O(n \log n)$ time.
  - A query is solved by a binary search which needs $O(\log n + m)$ time, where m is the (output-sensitive) number of points returned.
- Note, however, that an array-based solution is static and does not support insertions or deletions of points.
- Case $k \geq 2$:
  - There is no obvious way to generalize a solution based on sorting to $k \geq 2$ dimensions: The query time may be $O(n)$ even if no points of S lie within $\mathcal{R}$.
  - Still, the goal is to “extend” binary search to higher dimensions, ideally allowing dynamic updates.

Range Searching: kd-Tree

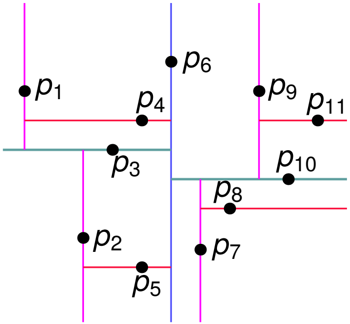
- For points $p_1, \ldots, p_n$ in $\mathbb{R}^2$ we build a kd-tree ("*k*-dimensional (binary search) tree") as preprocessing:
  - We start by finding the median p_m of the points with respect to their *x*-coordinates. (W.l.o.g.: "general position assumed!")
  - The point p_m becomes the root of the tree; it is labeled "vertical".
  - We divide the plane by a vertical straight line through p_m into two half-planes.

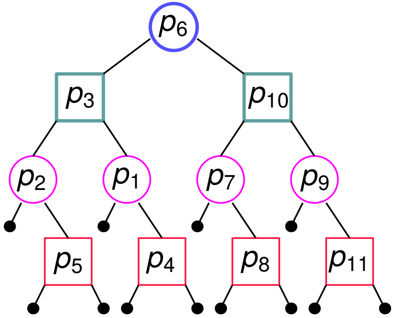




Range Searching: kd-Tree

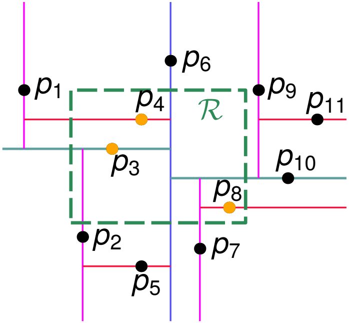
- For points $p_1, \ldots, p_n$ in $\mathbb{R}^2$ we build a kd-tree as the preprocessing:
  - Within each half-plane we find the medians with respect to the *y*-coordinates of the respective points.
  - These two points are called “horizontal” nodes and become the left and the right child of the root.
  - The recursive subdivision, alternating between *x*- and *y*-coordinates, continues until all points form nodes of the tree.

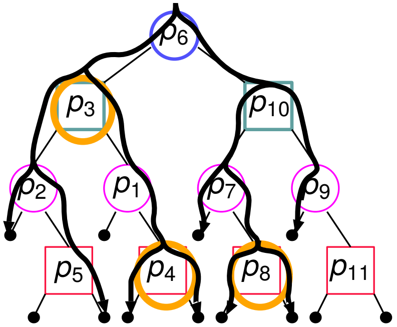




Range Search: kd-Tree Traversal

- Suppose that a query rectangle $\mathcal{R} := [x_1, x_2] \times [y_1, y_2]$ is given for $x_1, x_2, y_1, y_2 \in \mathbb{R}$ with $x_1 \le x_2$ and $y_1 \le y_2$.





Complexity of Range Searching Based on a kd-Tree

Theorem 147

Range searching based on a kd-tree in two dimensions needs $O(n \log n)$ preprocessing time, with $O(n)$ space complexity. A query can be carried out in $O(\sqrt{n} + m)$ time, where m is the number of nodes reported.

Sketch of Proof : We focus on the query complexity. Fix one supporting line ℓ of the query rectangle. W.l.o.g., ℓ is vertical. Let $Q^x(n)$ be the maximum number of nodes of the kd-tree which are discriminated relative to ℓ if the root of the kd-tree is split according to x-coordinate. Similarly for $Q^y(n)$. We get for ℓ being vertical:

$$Q^x(n) = 1 + Q^y\left(\frac{n}{2}\right) \qquad \text{and} \qquad Q^y(n) = 1 + 2Q^x\left(\frac{n}{2}\right).$$

Induction allows to show

$$Q^x(n) = 2 + 2Q^x\left(\frac{n}{4}\right).$$

The Master Theorem 32 tells us that $Q^x \in O(\sqrt{n})$ and, thus, also $Q^y \in O(\sqrt{n})$. (One could also prove directly $Q^x(n) \leq 3\sqrt{n} - 2$.) Hence, $O(\sqrt{n})$ nodes are discriminated relative to the four supporting lines of the query rectangle. □

Complexity of Range Searching Based on a kd-Tree

- The complexity of building a kd-tree does not change if no linear-time algorithm for median finding is used but pre-sorting is carried out. (Actually, it makes the implementation simpler.)
- For a range search in $\mathbb{R}^k$ we split the space alternatingly by straight lines ($k = 2$), planes ($k = 3$), or hyper-planes (for $k \geq 4$).

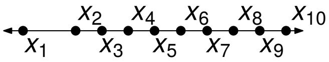
Theorem 148

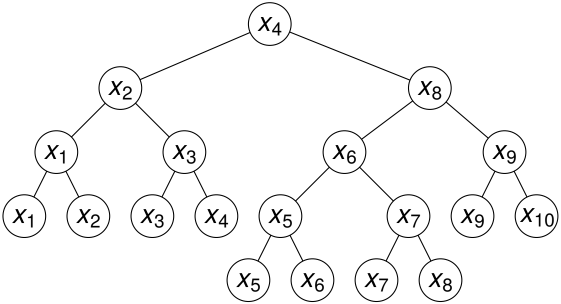
For a fixed dimension $k \geq 2$, range searching in $\mathbb{R}^k$ based on a kd-tree needs $O(n \log n)$ preprocessing time, with $O(n)$ space complexity. A query can be carried out in $O(n^{1-1/k} + m)$ time, where m is the number of nodes reported.

- Note the curse of dimensionality for large values of k!
- But kd-trees are a very versatile tool in low dimensions!

Range Tree in One Dimension

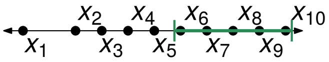
- We revisit range searching in one dimension:
  - Rather than sorting and storing the numbers in an array, we store them in a (balanced) binary search tree.
  - We use a leaf tree as BST: Every node has either zero or two children and only the leaves contain the data; every inner node stores the largest value of its left subtree.
- Such a BST on n items can be constructed in $O(n \log n)$.

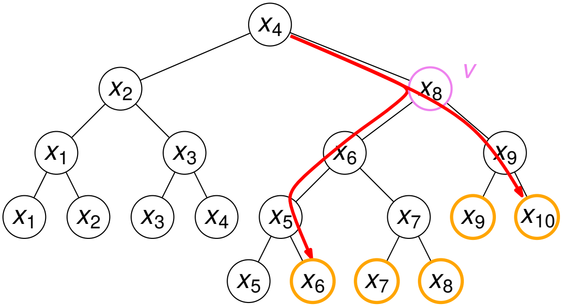




Range Tree in One Dimension

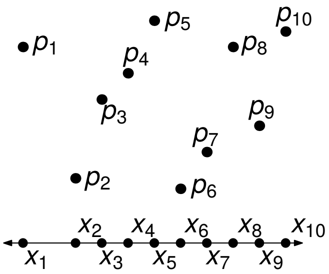
- For a query interval $[x', x'']$, we locate x' and x'' in the BST.
- Consider the "split node" v where the two paths to x' and x'' diverge.
- If the value stored in a node v' on the search path from v to the node located by x' is less than or equal to x' then report all leaves in the right subtree of v'. Similarly for left subtrees in the right search path after v.
- We get $O(m + \log n)$ as query time, where m is the number of items reported.
- Updates are possible in $O(\log n)$ time per update.



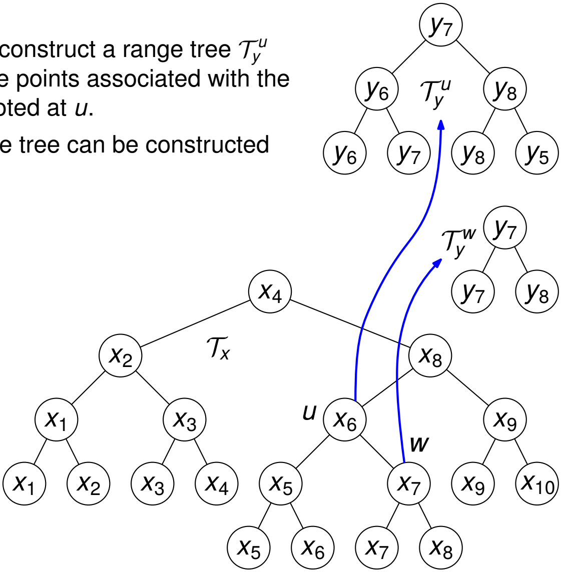


Range Tree in Two Dimensions

- Construct a one-dimensional range tree $\mathcal{T}_x$ relative to the x-coordinates of the points.
- For every inner node u of $\mathcal{T}_x$, construct a range tree $\mathcal{T}_y^u$ relative to y-coordinates of the points associated with the leaves of the subtree of $\mathcal{T}_x$ rooted at u.
- The full two-dimensional range tree can be constructed in $O(n \log^2 n)$ time in total.



p_1
p_2
p_3
p_4
p_5
p_6
p_7
p_8
p_9
p_{10}
x_1 x_2 x_3 x_4 x_5 x_6 x_7 x_8 x_9 x_{10}



Range Tree in Two Dimensions Refined

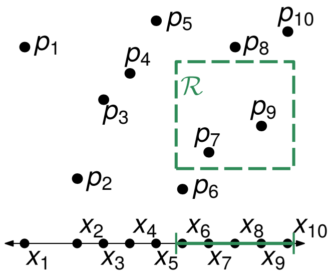
- It is easy to to construct a BST of $x_1, x_2, \ldots, x_n$ in $O(n)$ time if $x_1 < x_2 < \ldots < x_n$.
- Hence, in two dimensions we can proceed as follows:
  1. Sort the n points according to (1) their x-coordinates and (2) their y-coordinates.
  2. Renumber the points according to their x-order: $p_1, p_2, \ldots, p_n$.
  3. Make a root node v of a tree $\mathcal{T}_x$ for $p_{\lfloor n/2 \rfloor}$ and attach the range tree $\mathcal{T}_y^v$ (relative to y-coordinates) of $p_1, p_2, \ldots, p_n$ to it.
  4. Recursively generate two-dimensional range trees for $p_1, p_2, \ldots, p_{\lfloor n/2 \rfloor}$ and $p_{\lfloor n/2 \rfloor + 1}, \ldots, p_n$, and make them the left subtree and right subtree of $\mathcal{T}_x$ at v.
- We get $O(n \log n)$ for the construction of a range tree in two dimensions.
- This implies an $O(n \log n)$ bound on the memory consumption. (And, indeed, every leave of $\mathcal{T}_x$ shows up in $O(\log n)$ range trees relative to the y-coordinate.)

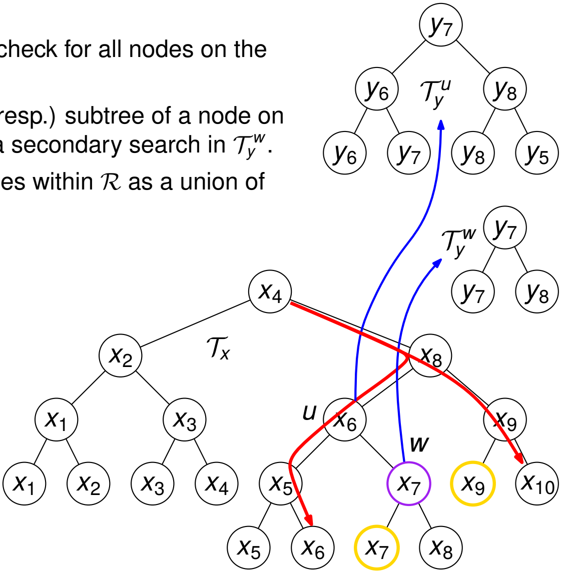
Lemma 149 (*Bentley (1979)*)

Range queries among n points of $\mathbb{R}^2$ can be answered in $O(m + \log^2 n)$ time. The construction of the range tree takes $O(n \log n)$ time and space.

Range Tree in Two Dimensions: Query

- For a query rectangle $\mathcal{R}$, perform a query relative to x-coordinates in $\mathcal{T}_x$.
- Containment in $\mathcal{R}$ is trivial to check for all nodes on the search paths.
- For the root w of a right (left, resp.) subtree of a node on the search path, we perform a secondary search in $\mathcal{T}_y^w$.
- This allows to identify the nodes within $\mathcal{R}$ as a union of disjoint sets of nodes.





$\mathcal{T}_y^u$
y_7 y_6 y_8 y_6 y_7 y_8 y_5
$\mathcal{T}_y^w$
y_7 y_7 y_8
$\mathcal{T}_x$
x_4 x_2 x_8 x_1 x_3 x_6 x_9
u
w
x_1 x_2 x_3 x_4 x_5 x_7 x_9 x_{10}
x_5 x_6 x_7 x_8

Range Tree in Higher Dimensions

Theorem 150 (*Bentley (1979)*)

For any fixed dimension $k \geq 2$, range queries among n points of $\mathbb{R}^k$ can be answered in $O(m + \log^k n)$ time. The generation of the range tree takes $O(n \log^{k-1} n)$ time and space.

Sketch of Proof: Generate a range tree for the first two dimensions in $O(n \log n)$ time and space, and recursively generate $O(\log n)$ range trees for $(k-2)$-dimensional space. □

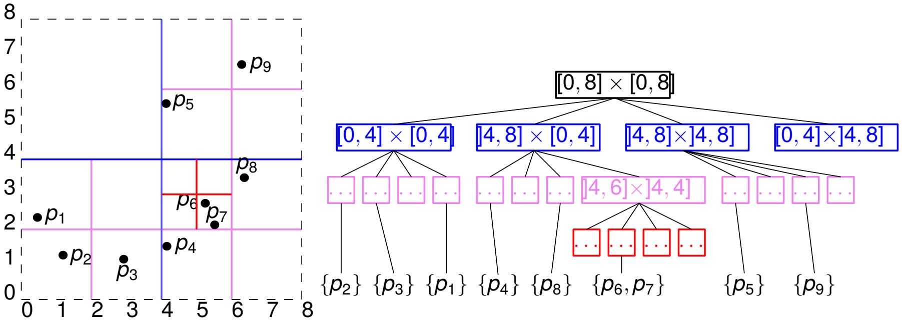
Theorem 151 (*Chazelle (1990)*)

The space complexity of a range tree in $k \geq 2$ dimensions can be reduced to $O\left(n \left(\frac{\log n}{\log \log n}\right)^{k-1}\right)$, and a query can be answered in $O(m + \log^{k-1} n)$ time.

- Range trees are an example for *multi-layer search trees*: multiple one-dimensional trees are layered to answer multi-dimensional range queries.

Quadtree

- Consider a bounding box of the points $p_1, \ldots, p_n$ in $\mathbb{R}^2$. E.g., pick $m_1, m_2 \in \mathbb{N}_0$ and transfer the points such that they fit into the workspace $[0, 2^{m_1}] \times [0, 2^{m_2}]$.
- We subdivide the (rectangular) workspace recursively into four sub-rectangles ("cells") by bisecting it in both x and y.
- The recursion stops when either a cell contains at most one point or a maximum depth — i.e., minimum cell size — is reached.



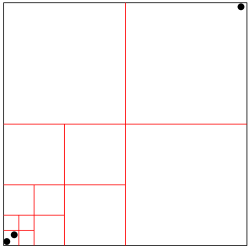
Quadtree

- Range queries in such a (point or point-region) quadtree are very similar to queries in a kd-tree.
- Insertion and deletion of points are supported easily.
- Quadtrees (Dt.: Quaternärbaum) are simple and easy to implement and tend to be quite efficient in practice.
- However, even just three points can result in a quadtree of huge height!
- Higher dimensions: In $\mathbb{R}^d$ we split into 2^d hyper-rectangles. When $d = 3$: *octree*.
- Rarely used for $d > 3$ and impractical for large d.

Theorem 152

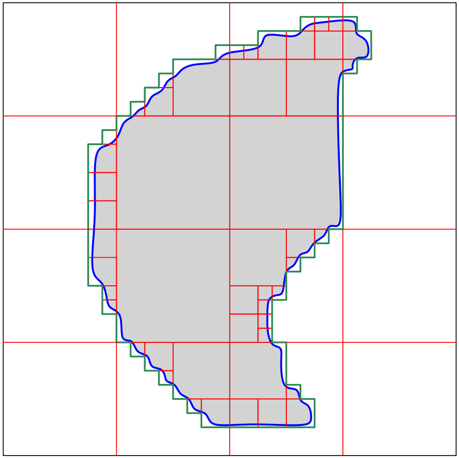
Consider a quadtree on the distinct points $p_1, p_2, \ldots, p_n$ such that every cell is either empty or contains at most one point. Then its height is in $O(\log \Delta)$, where

$$\Delta := \frac{\max_{1 \le i < j \le n} d(p_i, p_j)}{\min_{1 \le i < j \le n} d(p_i, p_j)}.$$



Quadtree

- Quadtrees and octrees are widely used for representing a shape approximately: *region quadtree* and *region octree*.



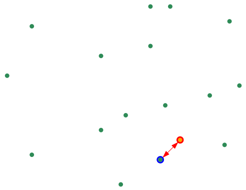
Nearest Neighbor Search

Problem: NEARESTNEIGHBORSEARCH

Input: A set S of n points in the Euclidean plane.

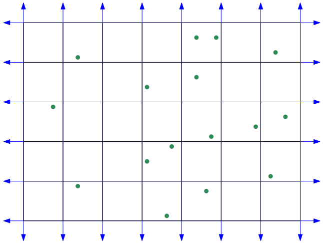
Output: The point of S which is closest to a query point q, for a given point q.

- We do already know that the worst-case complexity of NEARESTNEIGHBORSEARCH for n points has an $\Omega(\log n)$ lower bound.
- Easy to solve in $O(n)$ time per query.
- A worst-case optimum $O(\log n)$ query is possible, after $O(n \log n)$ preprocessing, based on tools of computational geometry.



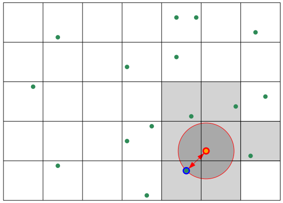
Geometric Hashing: Regular Rectangular Grid

- Let $S := \{p_1, p_2, \ldots, p_n\}$.
- The bounding box of S (or of a larger region that contains S) is partitioned into rectangular cells of uniform size by means of a regular grid.
- For every cell c, all points of S that lie in c are stored in a list associated with c.
- That is, the cells of the grid become the slots of the standard hash table, and the hash function assigns a point $p \in S$ to c if and only if p lies within c.
- We can cover the entire plane by extending boundary cells to infinity.



Geometric Hashing and Nearest Neighbor Search

- Determine the cell c in which the query point q lies.
- By searching in c (and possibly in its neighboring cells, if c is empty), we find a first candidate for the nearest neighbor.
- Let δ be the distance from q to this point.
- We continue searching in c and in those cells around c which are intersected by a disk D with radius δ centered at q.
- Whenever a point of S is found that is closer to q than δ, we reduce δ appropriately.
- The search stops once no unsearched cell exists that is intersected by the disk D.



Geometric Hashing: Grid Resolution

- What is a suitable resolution of the grid? There is no universally valid answer. In any case, the grid should not use more than $O(n)$ memory!

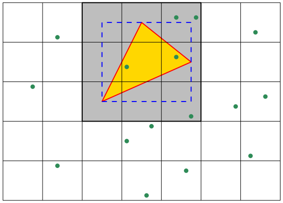
Personal experience

- Grids of the form $(w \cdot \sqrt{n}) \times (h \cdot \sqrt{n})$ seem to work nicely, with $w \cdot h = c$ for some constant c.
- The parameters w, h are chosen to adapt the resolution of the grid to the aspect ratio of the bounding box of the points.
- By experiment: $1 \leq c \leq 2$.

- This basic scheme can be tuned considerably:
  - Switch to multi-level hashing or to kd-trees if a small sample of the points indicates that the points are distributed highly non-uniformly.
  - Adapt the grid resolution and re-hash if the number of points stored changes significantly due to insertions and deletions of points.
- Hash-based nearest-neighbor searching will work best for points that are distributed uniformly, and will fail miserably if all points end up in one cell!
- Still, personal experience tells me that (tuned) geometric hashing works extremely well even for point sets that are distributed highly irregularly!

Geometric Hashing and Range Searching

- Geometric hashing can also be used to answer (generalized) range queries quite efficiently.
- E.g., one may need to report those points of S that lie within a query triangle.
- Then it suffices to check those points of S which are stored in cells overlapped by (the bounding box of) the triangle.



Hard Problems and Approximation Algorithms

Tractable vs. Intractable Problems

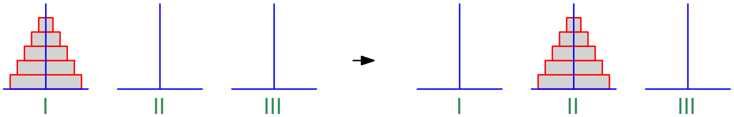
Definition 153 (*Polynomially solvable, Dt.: in polynomialer Zeit lösbar*)

A problem P is *solvable in polynomial time* if there exists a polynomial p such that a solution for every instance of P can be obtained in time $O(p)$, where the size of the instance/input forms the argument of the polynomial.

- Note: $O(n)$, $O(n \log^2 n)$, $O(2^{1000} n^3 \sqrt{n})$ and $O(n^{1000})$ all are polynomial bounds.
- A polynomial-time algorithm need not be practical: Even an $O(n^2)$ algorithm might already be impractical on realistic sizes of problems!
- Motivation for distinguishing between polynomial and non-polynomial problems:
  - If a problem is not solvable in polynomial time then there is absolutely no hope for an efficient (exact) solution for all large inputs. Such problems are considered *intractable*.
  - Polynomials have a nice closure property under standard operations: If p and q are polynomials then $p \odot q$ is a polynomial for most "standard" operations $\odot$.
  - If a problem of size n is solvable in time $f(n)$ on one model of computation then it is also solvable in time $f(p(n))$ on another model of computation, for virtually all "natural" models of computation and suitable polynomials p.

Sample Non-Polynomial Problem: Towers of Hanoi

- Tower-of-Hanoi Problem (ToH): Given three pegs (labeled I,II,III) and a stack of n disks arranged on Peg I from largest at the bottom to smallest at the top, we are to move all disks to Peg II such that only one disk is moved at a time and such that no larger disk ever is placed on a smaller disk.
- Attributed to Édouard Lucas [1883]. Supposedly based on an Indian legend about Brahmin priests moving 64 disks in the Great Temple of Benares; once they are finished, life on Earth will end.
- Goal: Find an algorithm that uses the minimum number of moves.



- One can prove: A (straightforward) recursive algorithm needs $2^n - 1$ moves.
- One can also prove: Every(!) algorithm that solves ToH needs at least $2^n - 1$ moves.
- Thus, the solution achieved by the recursive algorithm is optimal as far as the number of moves is concerned: No polynomial-time solution exists!
- [Buneman&Levy (1980)]: There exists a simple iterative solution that avoids an exponential-sized stack!

$\mathcal{P}$ and $\mathcal{NP}$

Definition 154 (*Problem Class $\mathcal{P}$*)

The problem class $\mathcal{P}$ is the class of all decision problems that are solveable in polynomial time by a deterministic algorithm.

- Intuitively, the class $\mathcal{NP}$ is the class of those decision problems for which one can verify on a deterministic computer in polynomial time whether or not an alleged solution (“certificate”) is indeed a correct solution that allows the algorithm to answer “yes”.
- For instance, while it appears difficult to assign colors to nodes of a graph such that the minimum amount of colors is used, it is easy to check (in polynomial time) whether a suggested assignment of colors yields a proper coloring.

$\mathcal{P}$ and $\mathcal{NP}$

- Often, $\mathcal{NP}$ is informally described as the class of decision problems that can be solved by a non-deterministic algorithm in polynomial time.
- Roughly, a non-deterministic algorithm consists of a "guessing" phase and a "verifying phase".
  1. Guessing: An arbitrary string s of characters is generated.
  2. Verifying: A deterministic algorithm takes the input and the string s. It may use or ignore s during its computation. Eventually, it returns the correct answer "yes" or "no", or it may get in an infinite loop and never halt.
- The time consumed by a non-deterministic algorithm is the time needed to write s plus the time consumed by the deterministic verifying phase.

Definition 155 (*Non-deterministic Polynomial-time Solution*)

A *non-deterministic algorithm solves a decision problem P in polynomial time* if there is a fixed polynomial p such that for every instance x of P for which the answer is "yes" there is at least one execution of the algorithm that returns "yes" in at most $p(|x|)$ time.

$\mathcal{P}$ and $\mathcal{NP}$

Definition 156 (*Problem Class $\mathcal{NP}$*)

The problem class $\mathcal{NP}$ is the class of all decision problems that are solveable in polynomial time by a non-deterministic algorithm.

$\mathcal{NP}$ . . .

. . . is not a short-hand for “not polynomial”!

- Note that being in $\mathcal{NP}$ does not imply for a problem that we can easily find a certificate s for an instance if the answer is “yes”. But there has to exist a polynomial-time algorithm to check the validity of a proposed certificate s.

Lemma 157

We have $\mathcal{P} \subseteq \mathcal{NP}$.

Sketch of Proof : Let $P \in \mathcal{P}$. All we need to do is to apply a deterministic algorithm that solves P in polynomial time and let it ignore any non-determinism. □

Polynomial Reducibility

Definition 158 (*Polynomially Reducible, Dt.: polynomial reduzierbar*)

A decision problem P is *polynomially reducible* (or simply *reducible*) to a decision problem Q, denoted by $P \leq_p Q$, if there exists a reduction from P to Q that runs in polynomial time.

- This definition can easily be extended to cover reductions from a decision problem P to an arbitrary problem Q by requesting that the output generated by an instance of Q allows to decide in polynomial time whether the answer for the original instance of P is “yes” or “no”.
- Such an extension allows a reduction from a combinatorial decision problem to a combinatorial optimization problem.

Lemma 159

For two decision problems P, Q, if $P \leq_p Q$ and $Q \in \mathcal{P}$ then $P \in \mathcal{P}$.

Proof : Let x be an instance of P. We apply a polynomial reduction and map x in time $p(|x|)$ to an instance $t(x)$ of Q. Since $Q \in \mathcal{P}$, a solution to $t(x)$ can be obtained in time $q(p(|x|))$, where $q(|\alpha|)$ denotes the time needed for solving an instance α of Q. □

Polynomial Reducibility: P-Complete

Definition 160 (*$\mathcal{P}$-complete, Dt.: $\mathcal{P}$-vollständig*)

A problem $P \in \mathcal{P}$ is $\mathcal{P}$-complete if $Q \leq_p P$ for every $Q \in \mathcal{P}$.

- $\mathcal{P}$-complete problems are widely assumed to be inherently sequential, i.e., very difficult to parallelize in any reasonable way.

$\mathcal{NP}$-Hardness and $\mathcal{NP}$-Completeness

Definition 161 (*$\mathcal{NP}$-hard, Dt.: $\mathcal{NP}$-schwer*)

A problem Q is $\mathcal{NP}$-*hard* if every problem $P \in \mathcal{NP}$ is polynomially reducible to Q.

- Note that $\mathcal{NP}$-hard does not mean "$\mathcal{NP}$ and hard"! Rather, it means "at least as hard as any problem in $\mathcal{NP}$".

Definition 162 (*$\mathcal{NP}$-complete, Dt.: $\mathcal{NP}$-vollständig*)

A problem Q is $\mathcal{NP}$-*complete* if it is in $\mathcal{NP}$ and if it is $\mathcal{NP}$-hard. The class of $\mathcal{NP}$-complete problems is denoted by $\mathcal{NPC}$.

- Hence, an optimization problem might be $\mathcal{NP}$-hard, but only decision problems can be $\mathcal{NP}$-complete.

Lemma 163

We have $\mathcal{NPC} \subseteq \mathcal{NP}$ and $\mathcal{NPC} \subset \mathcal{NP}$-hard.

$\mathcal{NP}$-Hardness and $\mathcal{NP}$-Completeness

Theorem 164 (*Cook (1971)*)

The satisfiability problem of propositional logic, SAT, is $\mathcal{NP}$-complete.

- Dt.: Erfüllbarkeitsproblem der Aussagenlogik.
- Which other problems are $\mathcal{NP}$-complete?
- [Karp (1972)]: He established the $\mathcal{NP}$-completeness of 21 combinatorial and graph-theoretical computational problems.
- See Garey and Johnson, "Computers and Intractability: A Guide to the Theory of $\mathcal{NP}$-Completeness". (This used to be the bible of $\mathcal{NP}$-completeness.)
- In the meantime, a few thousand problems are known to be $\mathcal{NP}$-complete . . .

A List of $\mathcal{NP}$-Complete Problems

Problem: SAT-CNF

Input: A propositional formula A which is in conjunctive normal form.

Decide: Is A satisfiable?

Problem: 3-SAT-CNF

Input: A propositional formula A which is in conjunctive normal form such that every clause consists of exactly (or at most) three literals.

Decide: Is A satisfiable?

Problem: SUBSETSUM, DT.: TEILSUMMENPROBLEM

Input: A set S of n natural numbers and a number $m \in \mathbb{N}$.

Decide: Does a subset of the numbers of S add up to exactly m?

Problem: BINPACKING, DT.: BEHÄLTERPROBLEM

Input: A set S of n objects with sizes $s_1, s_2, \ldots, s_n \in \mathbb{Q}$, where $0 < s_i \leq 1$, and a number $k \in \mathbb{N}$.

Decide: Do the objects fit into k bins of unit capacity?

A List of $\mathcal{NP}$-Complete Problems

Note

It is common not to make an explicit distinction between a decision problem, as listed, and its optimization variant (if it exists): For the optimization problem we drop "and a number k" and replace "decide" by "maximize k" or "minimize k". (We will also be liberal in using the same name both for a decision problem and for its optimization variant ...)

Problem: KNAPSACK (KNAP), DT.: RUCKSACKPROBLEM

Input: A knapsack of capacity $c \in \mathbb{N}$ and n objects with sizes $s_1, s_2, \dots, s_n$ and "profits" $p_1, p_2, \dots, p_n$. In addition, we are given a number $k \in \mathbb{N}$.

Decide: Is there a subset of the objects that fits into the knapsack and achieves a total profit of at least k?

Problem: SETCOVER (SC), DT.: MENGENÜBERDECKUNGSPROBLEM

Input: A set S and a family $\mathcal{S} := \{S_1, S_2, \dots, S_m\}$ of m subsets of S, for $m \in \mathbb{N}$, and a natural number $k \in \mathbb{N}$.

Decide: Do there exist at most k subsets $S_{i_1}, S_{i_2}, \dots, S_{i_k} \in \mathcal{S}$ such that $S = S_{i_1} \cup S_{i_2} \cup \dots \cup S_{i_k}$?

A List of $\mathcal{NP}$-Complete Problems

Problem: HAMILTONIANCYCLE (HC)

Input: An undirected graph $\mathcal{G}$.

Decide: Does $\mathcal{G}$ contain a Hamiltonian cycle?

Problem: HAMILTONIANPATH (HP)

Input: An undirected graph $\mathcal{G}$.

Decide: Does $\mathcal{G}$ contain a Hamiltonian path?

Problem: TRAVELINGSALESMANPROBLEM (TSP), DT.: RUNDREISEPROBLEM

Input: A weighted and undirected graph $\mathcal{G}$, and a number $c \in \mathbb{R}^+$.

Decide: Does $\mathcal{G}$ contain a Hamiltonian cycle whose total cost is less than c?

Problem: MINIMUMSTEINERTREE (MST), DT.: STEINERBAUMPROBLEM

Input: A weighted and undirected graph $\mathcal{G} = (V, E)$, a set of required nodes (“terminals”) $T \subset V$, and a number $c \in \mathbb{R}^+$.

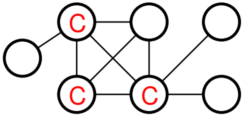
Decide: Does there exist a connected subgraph (V', E') of $\mathcal{G}$ such that $T \subseteq V'$ and the sum of the costs of the edges of E' is less than c?

A List of $\mathcal{NP}$-Complete Problems

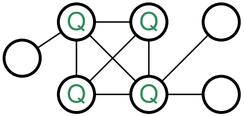
Problem: VERTEXCOVER (VC), DT.: KNOTENÜBERDECKUNGSPROBLEM

Input: An undirected graph $\mathcal{G} = (V, E)$ and a number $k \in \mathbb{N}$.

Decide: Does there exist a vertex cover that has k vertices? (A subset $C \subseteq V$ of the vertices of a graph $\mathcal{G}$ forms a vertex cover of $\mathcal{G}$ if every edge of E is incident upon at least one vertex of C.)



Vertex Cover



Clique

Problem: CLIQUE (CLIQ), DT.: CLIQUENPROBLEM

Input: An undirected graph $\mathcal{G} = (V, E)$ and a number $k \in \mathbb{N}$.

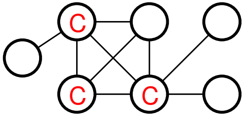
Decide: Does $\mathcal{G}$ have a clique of size k? (A subset $Q \subseteq V$ of the vertices of a graph $\mathcal{G}$ forms a clique of $\mathcal{G}$ if every pair of distinct vertices of Q is linked by an edge of E.)

A List of $\mathcal{NP}$-Complete Problems

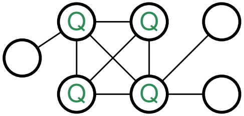
Problem: INDEPENDENTSET (IS), DT.: STABILITÄTSPROBLEM

Input: An undirected graph $\mathcal{G} = (V, E)$ and a number $k \in \mathbb{N}$.

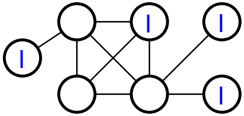
Decide: Does $\mathcal{G}$ have an independent set of size k? (A subset $I \subseteq V$ of the vertices of a graph $\mathcal{G}$ forms an independent set if no pair of vertices of I is connected by an edge of E.)



Vertex Cover



Clique



Independent Set

Problem: k-COLORING (k-COL), DT.: k-FÄRBBARKEIT

Input: An undirected graph $\mathcal{G} = (V, E)$, and an integer $k \in \mathbb{N}$.

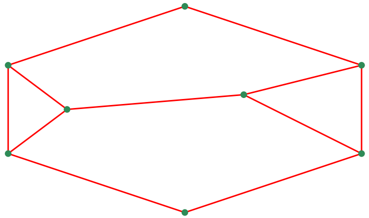
Decide: Does $\mathcal{G}$ admit a coloring that uses at most k colors? (An assignment of colors to all vertices of V is called a (vertex) coloring if adjacent vertices are assigned different colors.)

A List of $\mathcal{NP}$-Complete Problems: Minimum Convex Decomposition

Problem: MinimumConvexDecomposition (MCD)

Input: A set S of n points in the plane.

Output: A planar straight-line graph with vertex set S, with each point in S having positive degree, that partitions $CH(S)$ into the smallest possible number of convex faces.



- [Grelier (2020)]: MCD is $\mathcal{NP}$-hard.
- [Knauer&Spillner (2006)]: If no three points of S are collinear then a 3-approximation for MCD can be computed in $O(n \log n)$ time; a $^{30}/_{11}$-approximation can be computed in $O(n^2)$ time.
- [Eder et al. (2020)]: Engineering-based heuristics seem to achieve close-to-optimum solutions.

A List of $\mathcal{NP}$-Complete Problems: ETSP?

- Recall that TSP is $\mathcal{NP}$-complete.
- Intuitively, ETSP ought to be $\mathcal{NP}$-complete, too.
- Indeed, the $\mathcal{NP}$-completeness of ETSP is claimed in several publications . . .
- However, this claim is wrong! (The title of [Papadimitriou (1977)], "The Euclidean travelling salesman problem is $\mathcal{NP}$-complete", is misleading!)
- ETSP, and several other optimization problems involving Euclidean distance, are not known to be in $\mathcal{NP}$ due to a "technical twist": For ETSP, the length of a tour on n points (with integer/rational coordinates) is a sum of n square roots. Comparing this sum to a number c may require very high precision, and no polynomial-time algorithm is known for solving this problem.

Open problem

Can the sum of n square roots of integers be compared to another integer in polynomial time?

ETSP is $\mathcal{NP}$-hard . . .

. . . but not known to be in $\mathcal{NP}$.

A List of $\mathcal{NP}$-Complete Problems in CS

Theorem 165

The following decision problems are $\mathcal{NP}$-complete:

- SAT-CNF,
- 3-SAT-CNF,
- SUBSETSUM,
- BINPACKING,
- KNAPSACK,
- SETCOVER,
- HAMILTONIANCYCLE,
- HAMILTONIANPATH,
- TSP,
- MINIMUMSTEINERTREE,
- VERTEXCOVER,
- CLIQUE,
- INDEPENDENTSET,
- k-COL.

A List of $\mathcal{NP}$-Complete Problems in the Sciences

- $\mathcal{NP}$-completeness is not just a concern to theoreticians!
- Rather, many fundamental problems in the sciences have been shown to be $\mathcal{NP}$-complete (or $\mathcal{NP}$-hard).
- The following list was taken from “The status of the P versus NP problem” [Fortnow, CACM (2009)]:
  - Finding a DNA sequence that best fits a collection of fragments of the sequence [Gusfield (1997)].
  - Finding a ground state in the Ising model of phase transitions [Cipra (2000)].
  - Finding Nash Equilibriums with specific properties in a number of environments [Conitzer (2008)].
  - Finding optimal protein threading procedures [Lathrop (1994)].

$\mathcal{P} \neq \mathcal{NP}$?

Theorem 166

If some $\mathcal{NP}$-complete problem is in $\mathcal{P}$ then $\mathcal{P} = \mathcal{NP}$.

Proof: If an $\mathcal{NP}$-complete problem P is in $\mathcal{P}$, then all problems of $\mathcal{NP}$ can be reduced in polynomial time to P and, thus, also solved in polynomial time. □

Exponential Time Hypothesis [Impagliazzo&Paturi (1999, 2001)] . . .

. . . postulates that 3-SAT (and several other $\mathcal{NP}$-complete problems) cannot be solved deterministically in subexponential time.

- The exponential time hypothesis implies $\mathcal{P} \neq \mathcal{NP}$.
- But ETH is stronger than assuming $\mathcal{P} \neq \mathcal{NP}$!
- Want to become rich and famous? In 2000, the Clay Mathematics Institute (CMI) at Cambridge, Massachusetts (USA), named seven Millennium Prize Problems and designated a \$7 million prize fund for the solution of these problems, with \$1 million allocated to each problem. And the $\mathcal{P} = \mathcal{NP}$ question is one of them!

What $\mathcal{NP}$-Completeness Does Not Imply

- While all known $\mathcal{NP}$-complete problems are indeed tremendously difficult to solve, solving an $\mathcal{NP}$-complete problem does not “necessarily” require exponential time: Otherwise, ETH would be true and we would have $\mathcal{P} \neq \mathcal{NP}$!
- $\mathcal{NP}$-completeness does not imply that absolutely all (or even just most) instances of a problem are difficult. E.g., powerful SAT-solvers are known.
- $\mathcal{NP}$-complete problems are not the “most difficult” problems: They have a running time that is “only” exponential ...
- [Presburger (1929)] introduced a first-order theory of the natural numbers with addition and equality, but without multiplication. Its axioms include some form of induction. For every sentence in Presburger arithmetic one can decide, i.e., determine algorithmically, whether it follows from the axioms of Presburger arithmetic.
- [Fischer&Rabin (1974):] The decision algorithm for *Presburger arithmetic* for a sentence of length n has a worst-case running time of at least $2^{2^{c \cdot n}}$, for some constant $c > 0$.
- Algorithms with double exponential (worst-case) time also comprise the currently best known algorithms for computing a Gröbner basis and for quantifier elimination on real closed fields.

Proving $\mathcal{NP}$-Completeness of a Problem

Theorem 167

If $P \leq_p Q$ and P is $\mathcal{NP}$-complete and $Q \in \mathcal{NP}$ then Q also is $\mathcal{NP}$-complete.

Proof : Let R be in $\mathcal{NP}$. We reduce an instance x of R to an instance $t_1(x)$ of P, and reduce $t_1(x)$ to an instance $t_2(t_1(x))$ of Q. This reduction runs in polynomial time. Hence, every problem that is in $\mathcal{NP}$ can be reduced polynomially to Q. □

Steps to prove a problem Q to be $\mathcal{NP}$-complete

1. Show that $Q \in \mathcal{NP}$.
2. Pick a problem P that is known to be $\mathcal{NP}$-complete.
3. Construct (or prove the existence of) a polynomial reduction from P to Q.

- $\mathcal{NP}$-completeness proofs tend to make extensive use of "gadgets". The (fairly creative) process of designing such gadgets is sometimes called "gadgeteering."

Trevisan et al. (2000)

A *gadget* is a finite combinatorial structure which translates a given constraint of one (optimization) problem into a set of constraints of a second (optimization) problem.

Sample $\mathcal{NP}$-Completeness Proof: 4-COL

Lemma 168

If 3-COL is $\mathcal{NP}$-complete then 4-COL is $\mathcal{NP}$-complete.

Proof :

- Suppose that 3-COL is $\mathcal{NP}$-complete. We show that 3-COL $\leq_p$ 4-COL. (Clearly, 4-COL is in $\mathcal{NP}$.)
- Consider a graph $\mathcal{G} = (V, E)$. We transform $\mathcal{G}$ into a graph $\mathcal{G}' = (V', E')$ by adding a vertex $v \notin V$ to V. Also, we add edges from v to all nodes of V. That is,
  - $V' := V \cup \{v\}$, and
  - $E' := E \cup \{uv : u \in V\}$.
- This transformation can be carried out in time polynomial in the number of nodes and edges of $\mathcal{G}$.
- Since v consumes one color which cannot be used for any other node of $\mathcal{G}'$, the graph $\mathcal{G}$ is 3-colorable exactly if $\mathcal{G}'$ is 4-colorable. □

Corollary 169

If k-COL is $\mathcal{NP}$-complete for some $k \in \mathbb{N}$ then $(k+1)$-COL is $\mathcal{NP}$-complete.

Sample $\mathcal{NP}$-Completeness Proof: 3-COL

Theorem 170

3-COL is $\mathcal{NP}$-complete.

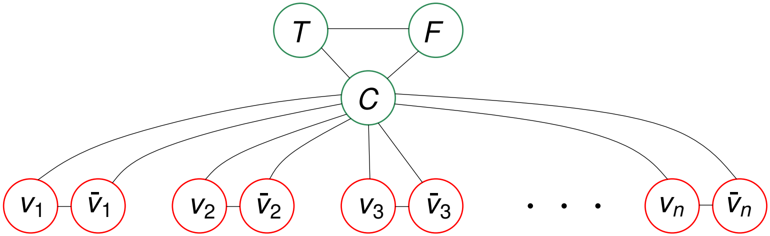
Proof:

- Clearly, 3-COL is in $\mathcal{NP}$. We prove 3-SAT-CNF $\leq_p$ 3-COL. Given a 3-CNF expression e, where every clause consists of exactly three literals, we show how to construct a graph $\mathcal{G}$ in polynomial time such that e is satisfiable if and only if $\mathcal{G}$ can be colored with three colors.
- Let k denote the number of clauses of e. The n variables appearing in e are denoted by $v_1, v_2, \ldots, v_n$.
- Hence, e contains at least one of the two literals v_i and $\bar{v}_i$, for all $i \in \{1, 2, \ldots, n\}$.
- We build an appropriate graph $\mathcal{G}$ that contains $2n + 6k + 3$ nodes and $3n + 12k + 3$ edges. This graph consists of
  - a graph representation of the variables, denoted by $\mathcal{G}_V$,
  - a graph representation of all clauses, $\mathcal{G}_C$, and of
  - appropriate edges to link $\mathcal{G}_V$ and $\mathcal{G}_C$ together.

Sample $\mathcal{NP}$-Completeness Proof: 3-COL

Proof of Thm. 170 (cont'd) :

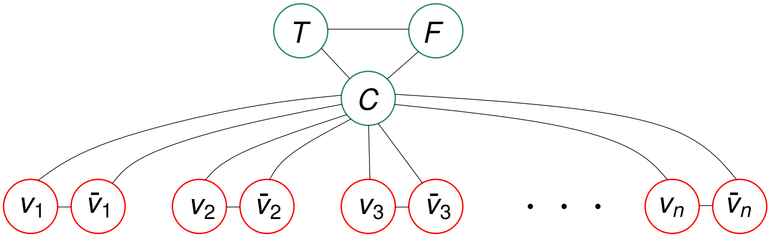
- Construction of $\mathcal{G}_V$ (to represent the variables):
  - Three special nodes — denoted by C (for "control"), T (for "true"), and F (for "false") — are linked into a triangle, the so-called control triangle.
  - For each variable v we create two nodes — the "literal nodes" v and $\bar{v}$ — and link them with the node C and with each other to form a triangle.
  - This gives $2n + 3$ nodes and $3n + 3$ edges constructed so far for $\mathcal{G}_V$.



Sample $\mathcal{NP}$-Completeness Proof: 3-COL

Proof of Thm. 170 (cont'd) :

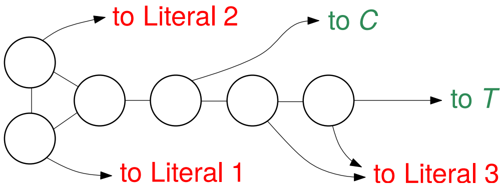
- Clearly, three colors are necessary and sufficient to color $\mathcal{G}_V$.
- Due to the use of the control node C, the variable nodes v_i and $\bar{v}_i$ have to use the same colors as the nodes T and F.
- If the colors of v_i and T match, then the colors of $\bar{v}_i$ and F have to match, too.
- Intuitively, think of assigning the variable v_i the value *true* if its node is colored with the same color as T. Similarly, coloring v_i with the same color as F can be interpreted as assigning the value *false* to v_i, thus, assigning the value *true* to $\bar{v}_i$.



Sample $\mathcal{NP}$-Completeness Proof: 3-COL

Proof of Thm. 170 (cont'd) :

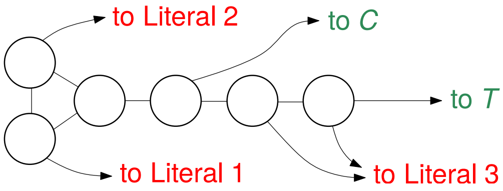
- Construction of $\mathcal{G}_C$ (to represent the clauses):
  - We use a clause gadget as depicted below, with one gadget per clause.
  - Each clause gadget is linked to five other nodes of $\mathcal{G}_V$:
    1. It is linked to the nodes C and T of the control triangle, and
    2. to three literal nodes corresponding to the literals that appear in the specific clause represented by the clause gadget.
  - The graph $\mathcal{G}_C$ is formed by k copies of this gadget, with one gadget per clause, resulting in a total of $6k$ additional nodes and $12k$ additional edges.



Sample $\mathcal{NP}$-Completeness Proof: 3-COL

Proof of Thm. 170 (cont'd) :

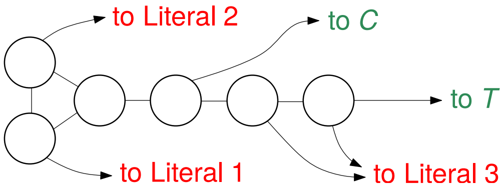
- The final graph $\mathcal{G}$ consists of $\mathcal{G}_V$ plus $\mathcal{G}_C$, i.e., of $2n + 6k + 3$ nodes and $3n + 12k + 3$ edges. Clearly, $\mathcal{G}$ can be constructed in time polynomial in the number of variables and clauses of e.
- Let a, b, c be the literal nodes that are pointed at by the three edges of a clause gadget marked by "to Literal . . .".
- Since a, b, c are linked to C, the only colors feasible for a, b, c are the two colors used for T and F.
- A simple enumeration of all possible color assignments to a, b, c shows that a clause gadget can be colored with three colors if and only if at least one of a, b, c is colored with the same color as T.



Sample $\mathcal{NP}$-Completeness Proof: 3-COL

Proof of Thm. 170 (cont'd) :

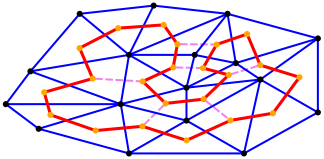
- We conclude that $\mathcal{G}$ can be colored with three colors exactly if there exists a consistent color assignment to all literal nodes such that at least one literal node of each clause is colored with the same color as T.
- Thus, the Boolean expression e is satisfiable if and only if $\mathcal{G}$ can be colored with three colors. □



Sample $\mathcal{NP}$-Completeness Proof: Hamiltonian Triangulation

Definition 171 (*Hamiltonian triangulation*)

A triangulation (of points or of polygonal figures) is *Hamiltonian* if its dual graph admits a Hamiltonian cycle.



Theorem 172 (*Arkin et al. (1996)*)

Testing whether a given simple polygon has a Hamiltonian triangulation can be done in $O(|E|)$ time, where $|E|$ is the number of visibility graph edges in the polygon.

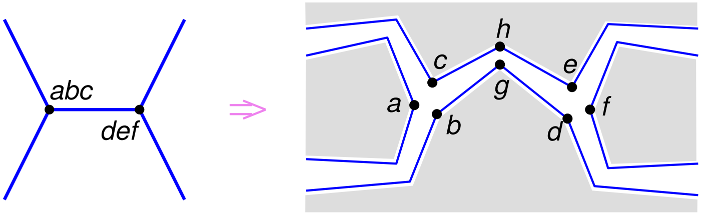
Theorem 173 (*Arkin et al. (1996)*)

Given a simple polygon with (simple polygonal) holes, it is $\mathcal{NP}$-complete to determine whether there exists a Hamiltonian triangulation of its interior.

Sample $\mathcal{NP}$-Completeness Proof: Hamiltonian Triangulation

Proof of Thm. 173 :

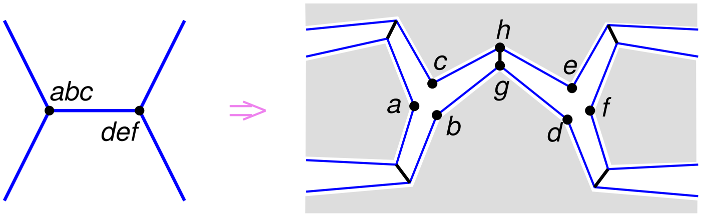
- We prove this theorem by reducing the known $\mathcal{NP}$-complete problem of determining whether a planar cubic graph is Hamiltonian to it. (Obviously, deciding whether such a triangulation exists is in $\mathcal{NP}$.)
- Given a straight-line plane drawing of a planar cubic graph $\mathcal{G}$, we construct a polygon with holes, where the holes correspond to the bounded faces of $\mathcal{G}$:
  - Each arc of $\mathcal{G}$ is mapped to a narrow "V"-shaped tunnel.
  - Thus, a node *abc* of $\mathcal{G}$ corresponds to three *node-vertices* *a*, *b*, *c* of the polygonal area.
  - Each arc of $\mathcal{G}$ introduces two *arc-vertices*, *g*, *h*, of the polygonal area.



Sample $\mathcal{NP}$-Completeness Proof: Hamiltonian Triangulation

Proof of Thm. 173 (cont'd) :

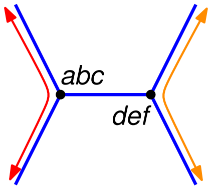
- We can construct the "V"-shaped tunnels such that the following properties hold:
  - The resulting polygons are simple and bound a polygonal area *P* with *k* holes if $\mathcal{G}$ contained *k* bounded faces.
  - A node-vertex is visible by another node vertex exactly if both correspond to the same node of $\mathcal{G}$.
  - Every arc-vertex sees exactly its corresponding arc-vertex and the corresponding six node-vertices.
  - Pairs of arc-vertices form *forced diagonals* contained in every triangulation.
- This construction can be carried out in polynomial time.



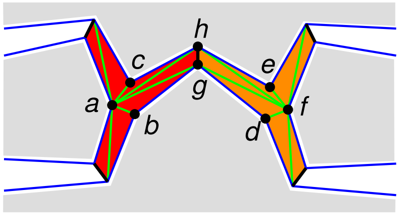
Sample $\mathcal{NP}$-Completeness Proof: Hamiltonian Triangulation

Proof of Thm. 173 (cont'd) :

- Suppose that $\mathcal{G}$ admits a Hamiltonian cycle.
- One can show that there exists a triangulation of P that is Hamiltonian.
- Now suppose that P has a triangulation that is Hamiltonian.
- One can show that $\mathcal{G}$ contains a Hamiltonian cycle.
- Recall that every triangulation contains the forced diagonals defined by the arc-vertices, which can be crossed by a Hamiltonian cycle at most once.
- Hence, the arcs of $\mathcal{G}$ that correspond to forced diagonals that the cycle crosses once in the triangulation of P form a Hamiltonian cycle in $\mathcal{G}$.
- Summarizing, $\mathcal{G}$ contains a Hamiltonian cycle if and only if P admits a Hamiltonian triangulation. $\square$



$\Leftarrow$



Dealing with $\mathcal{NP}$-Hard Problems

- Many combinatorial optimization problems could be solved by a brute-force enumeration of all possibilities.
- E.g., we could solve ETSP for n cities by enumerating all $(n-1)!$ possible tours.
- According to legend, the power of exponential growth was already known by the Brahmin Sissa ibn Dahir (ca. 300-400 AD): As a reward for the invention of the game of chess (or its Indian predecessor Chaturanga) he asked his king, Shihram, to place one grain of rice in the first square of a chessboard, two in the second, four in the third, and so on, doubling the amount of rice up to the 64-th square. Needless to say, the king could not fulfill Sissa's request . . .
- In short terms: An algorithm whose running time is 2^n or worse is all but useless for most practical applications!!
- Unfortunately, while proving a problem to be $\mathcal{NP}$-hard/complete might constitute quite an achievement, it tends to shed little light on how to solve it.
- So, what shall we do next?
- In the sequel, we will study algorithms that provide an approximation of the solution sought.
- But we will not just dive into heuristics: Our approximations will come with some guarantee of how far off they may be from the true solutions!

Constant-Factor Approximation

Definition 174 (*Approximation with guaranteed quality*)

For an instance I of an optimization problem, let $APX(I) > 0$ denote the numerical quantity achieved by an algorithm $\mathcal{A}$ that solves it approximately, and let $OPT(I) > 0$ denote the true optimum. Let $p\colon \mathbb{N} \to \mathbb{R}^+$. Then the approximation $\mathcal{A}$ has *quality p* if

$$\max\left\{\frac{APX(I)}{OPT(I)}, \frac{OPT(I)}{APX(I)}\right\} \le p(n)$$

holds for all input instances I of size n.

- Of course, $p(n) \ge 1$ for all $n \in \mathbb{N}$.

Note: *OPT* is unknown!

If we want to argue that some approximation algorithm has a particular guaranteed quality then we need to do so without knowing *OPT*!

Definition 175 (*Constant-factor approximation*)

An approximation algorithm with quality $p\colon \mathbb{N} \to \mathbb{R}^+$ is a *constant-factor approximation* with approximation factor $c \in \mathbb{R}^+$ if $p(n) \le c$ holds for all (sufficiently large) $n \in \mathbb{N}$.

Polynomial-Time Approximation Scheme

Definition 176 (*Polynomial-time approximation scheme (PTAS)*)

A *polynomial-time approximation scheme (PTAS)* for an optimization problem is an algorithm which takes as additional input a parameter $\varepsilon \in \mathbb{R}^+$ and generates a $(1+\varepsilon)$-approximation for every instance of the optimization problem such that its running time is a polynomial in n for problem instances of size n, for every fixed value of ε.

- Dt.: Polynomialzeitapproximationsschema.
- Common to PTAS algorithms is the fact that $O(1/\varepsilon)$ is allowed to appear as exponent of n or $\log n$.
- We may even see complexity terms of the form $O(n^{\lceil 1/\varepsilon \rceil !})$.
- A variant that is more useful in practice is a *fully polynomial-time approximation scheme* (FPTAS), for which we demand the time to be polynomial in both n and ${}^1/_\varepsilon$.
- *Quasi-polynomial-time approximation scheme* (QPTAS): We get a complexity of $O(n^{\text{polylog}\, n})$ for every fixed $\varepsilon \in \mathbb{R}^+$.

Approximate SetCover

Theorem 177

Consider a set S with n elements and a family $\mathcal{S} := \{S_1, S_2, \ldots, S_m\}$ of m subsets of S, with $\bigcup_{1 \le i \le m} S_i = S$. Then the following algorithm achieves an $(\ln n)$-approximation:

```
    Repeat until all elements of S are covered:
        Pick the set S_i with the largest number of uncovered elements.
```

Proof: Since it is obvious that the greedy algorithm achieves a cover, we focus on the approximation factor. Suppose that k sets of $\mathcal{S}$ suffice to cover S.
Let n_i be the number of elements of S not yet covered after the i-th iteration of the algorithm, with $n_0 := n$.
Since k sets suffice to cover also these remaining elements, one set (not yet picked by the algorithm) must exist in $\mathcal{S}$ that contains at least n_i/k of them. This implies

$$n_{i+1} \le n_i - \frac{n_i}{k} = n_i \left(1 - \frac{1}{k}\right) \le \ldots \le n_0 \left(1 - \frac{1}{k}\right)^{i+1}.$$

The standard inequality $1 - x < e^{-x}$, for all $x \in \mathbb{R} \setminus \{0\}$, implies

$$n_i \le n_0 \left(1 - \frac{1}{k}\right)^i < n_0 (e^{-1/k})^i = n \cdot e^{-i/k}.$$

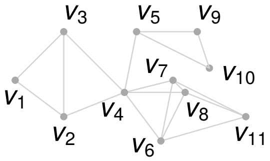
Since $n \cdot e^{-\ln n} = 1$, we get $n_i < 1$ (and no uncovered elements) for $i := k \ln n$. □

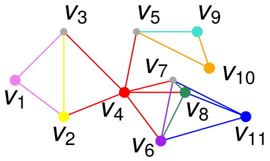
Approximate SETCOVER

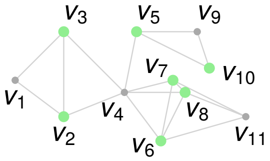
- [Slavík (1997)]: Tighter analysis yields $\ln n - \ln\ln n + \Theta(1)$ as approximation factor.
- [Lund&Yannakakis (1994), Feige (1998), Moshkovitz (2015)]: If $\mathcal{P} \neq \mathcal{NP}$ then it is impossible to devise a polynomial-time approximation algorithm for SETCOVER with approximation ratio $(1-\alpha)\ln n$, for any constant $\alpha > 0$.

Approximate VERTEXCOVER

- VERTEXCOVER can be seen as a special case of SETCOVER and, thus, has an $(\ln n)$-approximation by a simple greedy algorithm: Repeatedly delete the vertex of highest degree (and all incident edges).
- Suppose that we want to re-organize fire fighting and establish fire stations within some or all villages of a set of villages $V := \{v_1, v_2, \dots, v_n\}$ such that the driving distance between each village of V and its closest fire station is at most 15 km.







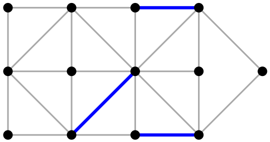
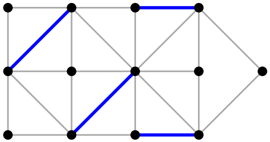
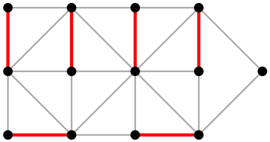
- Hence, the greedy algorithm yields eight fire stations while seven stations would also suffice.

Approximate VERTEXCOVER: Matching

Definition 178 (*Matching, Dt.: Paarung*)

- A *matching* in a simple graph $\mathcal{G} = (V, E)$ is a subset E' of E such that no two edges of E' are incident upon the same vertex of V.
- A *maximal matching* is a matching that does not allow to add an additional edge.
- A *maximum matching* is a matching with the largest-possible number of edges.
- A *perfect matching* is a matching that leaves no vertex unmatched.

- Of course, a perfect matching can only exist if $\mathcal{G}$ has an even number of nodes.
- If $\mathcal{G}$ is weighted then we seek matchings that minimize the sum of the edge weights.

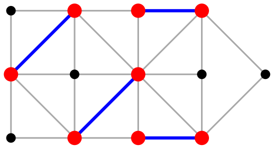
Approximate VERTEXCOVER

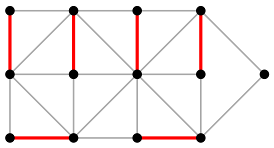
Theorem 179

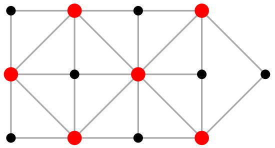
The vertices of all edges of a maximal matching of $\mathcal{G}$ yield a vertex cover with at most twice the number of vertices than optimum.

Proof : Let k_{max} be the number of edges of a maximum matching M of $\mathcal{G}$. Since every edge of M requires one vertex to cover it, any vertex cover of $\mathcal{G}$ contains at least k_{max} vertices.
On the other hand, we obtain a vertex cover by taking both end-points of every edge of any maximal matching of $\mathcal{G}$. Such a matching has k edges, with $k \leq k_{max}$. Hence, any maximal matching of $\mathcal{G}$ yields a vertex cover of $\mathcal{G}$ with at most $2k_{max}$ vertices. □

- The sample graph has a minimum vertex cover with six vertices.







Approximate ETSP

Lemma 180 (*Doubling-the-EMST heuristic*)

In $O(n \log n)$ time one can achieve an approximation of ETSP for n cities with approximation factor 2.

Lemma 181 (*Christofides (1976)*)

In $O(n^3)$ time one can achieve an approximation of ETSP for n cities with approximation factor $^3/_2$.

Theorem 182 (*Arora (1996), Mitchell (1996), Rao&Smith (1998)*)

There exists a polynomial-time approximation scheme for solving ETSP with approximation factor $(1+\varepsilon)$ in time $n^{O(1/\varepsilon)}$.

Approximate TSP

Metric TSP

The doubling-the-EMST approach works for any complete weighted graph $\mathcal{G} = (V, E)$ if the weights of the edges of $\mathcal{G}$ satisfy the triangle inequality:

$$c(u, v) \leq c(u, w) + c(w, v) \quad \text{for all } u, v, w \in V,$$

where $c(x, y)$ denotes the weight of the edge (x, y).

- The TSP problem becomes much harder to approximate if we deal with settings that do not satisfy the triangle inequality! For several settings we do not have polynomial-time approximations or cannot go beyond some approximation factor, unless $\mathcal{P} = \mathcal{NP}$.

Theorem 183

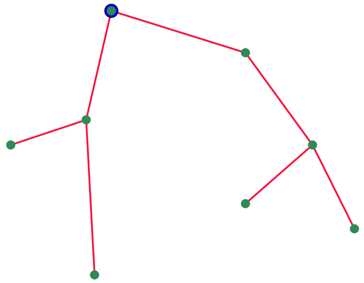
Let $p \colon \mathbb{N} \to \mathbb{N}$ be a polynomial-time computable function. Unless $\mathcal{P} = \mathcal{NP}$ there is no polynomial-time algorithm that outputs a solution of cost at most $p(n) \cdot OPT(I)$ for every TSP instance I of size n.

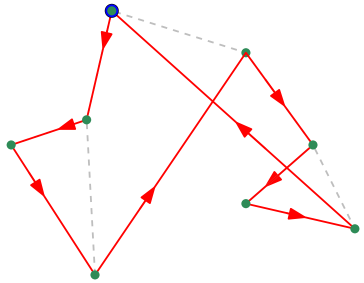
Approximate ETSP: Doubling-the-EMST Heuristic

Sketch of Proof of Lem. 180 :

1. Compute the Euclidean minimum spanning tree $\mathcal{T}(S)$ of S.
2. Select an arbitrary node v of $\mathcal{T}(S)$ as root.
3. Compute a (pre-order-like) traversal of $\mathcal{T}(S)$ rooted at v to obtain a tour $\mathcal{C}(S)$.
4. By-pass points already visited, thus shortening $\mathcal{C}(S)$.
5. Apply 2-opt moves (at additional computational cost).

- Time complexity: $O(n \log n)$ for computing the EMST $\mathcal{T}(S)$.
- Factor of approximation: $c = 2$ (even without Step 5). $\square$



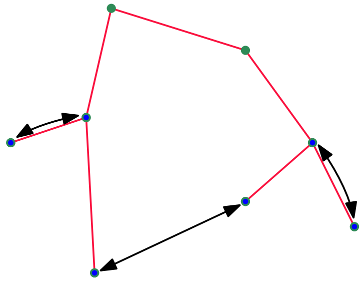


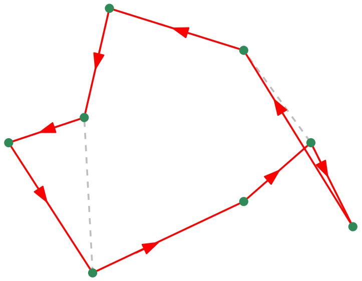
Approximate ETSP: Christofides' Heuristic

Sketch of Proof of Lem. 181 :

1. Compute the Euclidean minimum spanning tree $\mathcal{T}(S)$ of S.
2. Get a minimum Euclidean matching $\mathcal{M}$ on the vertices of odd degree in $\mathcal{T}(S)$.
3. Compute an Eulerian tour $\mathcal{C}$ on $\mathcal{T} \cup \mathcal{M}$.
4. By-pass points already visited, thus shortening $\mathcal{C}$.
5. Apply 2-opt moves (at additional computational cost).

- Time complexity: $O(n^3)$ for computing $\mathcal{M}$ [Edmonds (1965), Gabow (1972)].
- Factor of approximation: $c = \frac{3}{2}$ (even without Step 5). □





Problems of Unknown Complexity

- There are problems which are in $\mathcal{NP}$ but which are not known to be in $\mathcal{P}$ or to be $\mathcal{NP}$-complete.

Theorem 184 (*Ladner (1975)*)

If $\mathcal{P} \neq \mathcal{NP}$ then there exist problems in $\mathcal{NP}$ that are neither in $\mathcal{P}$ nor $\mathcal{NP}$-complete. These problems are called $\mathcal{NP}$-*intermediate*.

- Very few problems are of unknown complexity.

Problem: GRAPHISOMORPHISM

Input: Two (directed) graphs $\mathcal{G}_1$ and $\mathcal{G}_2$.

Decide: Is $\mathcal{G}_1$ isomorphic to $\mathcal{G}_2$?

- No polynomial-time algorithm is known for the graph isomorphism problem, but the problem is also not known to be $\mathcal{NP}$-complete.
- In the end of 2015, Babai announced a deterministic algorithm that runs in time $2^{O(\log^c n)}$ time for some positive constant c, i.e., in quasi-polynomial time.
- [Helfgott (2017)]: Claims that $c := 3$ is fine.

Problems of Unknown Complexity

Problem: **INTEGERFACTORIZATION**

Input: Two numbers $n, k \in \mathbb{N}$.

Decide: Does n have a factor less than (or greater than) some input k?

Problem: **DISCRETELOGARITHMPROBLEM (DLP)**

Input: Three numbers $a, b, k \in \mathbb{N}$.

Decide: Does the equation $a^x = b$ have a solution x over some (finite) group that is less than or greater than some input k.

- [Shor (1997)]: DLP can be solved on a hypothetical quantum computer in polynomial time.

Problem: **MINIMUMCIRCUITSIZEPROBLEM (MCSP)**

Input: A truth table of an unknown propositional formula and a number $k \in \mathbb{N}$.

Decide: Does there exist a propositional formula of size k that represents the truth table given?

3SUM-Hard Problems

Problem: 3SUM

Input: A set $S \subset \mathbb{Z}$ of n integers.

Decide: Does S contain three elements $a, b, c \in S$ such that $a + b + c = 0$?

- 3SUM was introduced by Gajentaan and Overmars (in a computational geometry paper) in 1995.
- One can solve 3SUM in $O(n^2)$ time by means of a clever sorting-based strategy.

Definition 185 (*3SUM-Hard*)

A problem P is called 3SUM-*hard* if 3SUM can be reduced to P in subquadratic time.

- Several seemingly unrelated problems are known to be 3SUM-hard.
- [Grønlund&Pettie (2014):] 3SUM can be solved in $O\left(n^2 / \left(\frac{\log n}{\log\log n}\right)^{2/3}\right)$ time!
- Still, no $O(n^{2-\varepsilon})$ solution is known for 3SUM, for any $\varepsilon \in \mathbb{R}^+$.

Linear and Integer Linear Programming

Linear Program

Problem: LINEARPROGRAM (LP, DT.: LINEARE OPTIMIERUNG)

Input: Vectors $b \in \mathbb{R}^n$ and $c \in \mathbb{R}^d$, and a matrix $\mathbf{A} \in M_{n \times d}$, for $d, n \in \mathbb{N}$.

Output: A solution vector $x \in \mathbb{R}^d$ such that

$$\mathbf{A}x \leq b \quad \text{and} \quad \langle c, x \rangle = \max\{\langle c, y \rangle : y \in \mathbb{R}^d \wedge \mathbf{A}y \leq b\}.$$

- Short-hand alternate formulations:
  - Maximize $\langle c, x \rangle$ subject to $\mathbf{A}x \leq b$.
  - Maximize $c^T x$ subject to $\mathbf{A}x \leq b$.
- We can use "minimize" instead of "maximize", and "$\geq$" or "$=$" instead of "$\leq$".
- Sample linear program:

$$\begin{array}{ll} \text{maximize:} & x_1 + 2x_2 \\ \text{subject to:} & x_2 \leq 4 \\ & x_2 \geq 1 \\ & 5x_1 - 4x_2 \leq 34 \\ & x_1 + x_2 \geq 4 \\ & 3x_1 + x_2 \leq 25 \end{array}$$

- $\mathbf{A} = \begin{pmatrix} 0 & 1 \\ 0 & -1 \\ 5 & -4 \\ -1 & -1 \\ 3 & 1 \end{pmatrix}$
- $c^T = (1, 2) \qquad x^T = (x_1, x_2)$
- $b^T = (4, -1, 34, -4, 25)$

Linear Program: Sample Problem

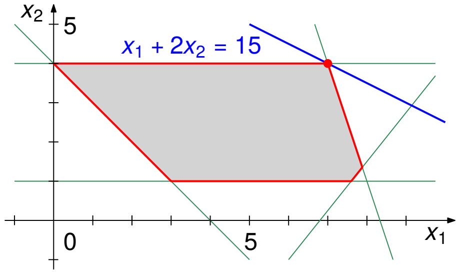
- A company produces two types of paint: exterior and interior paint.
- It makes a profit of € $3000(x_1 + 2x_2)$ if it produces x_1 tons of exterior paint and x_2 tons of interior paint.
- The set-up makes it necessary to produce at least 1 ton and at most 4 tons of interior paint per production cycle.
- For production reasons, the combined output has to be at least 4 tons of paint.
- One ton of exterior paint consumes 3 liters of a special liquid, while one ton of interior paint requires only 1 liter of that liquid, with 25 liters being available for one production cycle.
- Marketing considerations dictate $5x_1 - 4x_2 \leq 34$.

- Sample linear program:

$$\begin{array}{ll} \text{maximize:} & x_1 + 2x_2 \\ \text{subject to:} & \begin{array}{rcr} x_2 & \leq & 4 \\ x_2 & \geq & 1 \\ 5x_1 - 4x_2 & \leq & 34 \\ x_1 + x_2 & \geq & 4 \\ 3x_1 + x_2 & \leq & 25 \end{array} \end{array}$$

- Various real-world applications, ranging from business and economics to manufacturing and engineering. E.g.:
  - stock and asset management,
  - transport and energy optimization,
  - routing,
  - scheduling and assignment planning,
  - (network) flow optimization.

Linear Program: Geometric Interpretation



- Sample linear program:

  maximize: $x_1 + 2x_2$

  subject to:
  $$\begin{aligned} x_2 &\leq 4 \\ x_2 &\geq 1 \\ 5x_1 - 4x_2 &\leq 34 \\ x_1 + x_2 &\geq 4 \\ 3x_1 + x_2 &\leq 25 \end{aligned}$$

- Algorithm for solving LP for $d = 2$ manually:
  1. Graph all constraints as half-planes, thus obtaining the *feasible region*.
  2. Graph the objective function as a "movable" line.
  3. Find extreme point of feasible region in direction of objective function.

Linear Program: Basic Properties

- Every constraint models a half-plane (for $d = 2$) or a half-space (for $d \geq 3$).
- The feasibility region is given by the intersection of these regions.
- Hence, the feasibility region is a convex set: It can be
  - empty,
  - unbounded,
  - bounded.
- The objective function models a line (for $d = 2$) or a (hyper-)plane (for $d \geq 3$).
- If the feasibility region is bounded then an optimum solution is assumed in a vertex of the feasibility region.
- Even an unbounded feasibility region may result in a unique optimum solution.

Linear programming . . .

. . . has nothing to do with programming in today's meaning of the word "programming".

Negative variables

Some authors and some LP codes demand non-negative variables. In such a case $x_i \in \mathbb{R}$ can be modeled as $x_i = x_i' - x_i''$ with $x_i', x_i'' \in \mathbb{R}_0^+$.

Linear Program: How to Solve It

Simplex algorithm by Dantzig (1947).

- Matrix manipulation based on Gaussian elimination.
- Exponential worst-case complexity — see Klee-Minty cube in $\mathbb{R}^d$ — but fast in practice.
- It remains an open question whether there is a variation of the simplex algorithm that runs in time polynomial in only n and d.

Ellipsoid algorithm by Khachiyan (1979).

- First (weakly) polynomial-time algorithm for LP.
- No practical relevance.

Interior-point method by Karmarkar (1984).

- Runs in (weakly) polynomial time, too; quite efficient in practice.
- Several more recent IPM variants.

Ready-to-use software: Fierce competition between IPM and simplex methods has led to extremely fast LP solvers:

- GLPK (GNU Linear Programming Kit)
- CPLEX (IBM ILOG CPLEX Optimization Studio)
- MINOS
- GUROBI
- Mathematica, Maple, AMPL, . . .

Computation of Feasibility Region

Theorem 186

Randomized incremental construction allows to compute the intersection of n half-planes in $\mathbb{R}^2$ in $O(n)$ expected time.

Corollary 187

A (bounded) LP in $\mathbb{R}^2$ with n constraints can be solved in $O(n)$ expected time.

Theorem 188 (*Preparata&Muller (1979)*)

The intersection of n half-spaces in $\mathbb{R}^3$ can be computed (deterministically) in $O(n \log n)$ time.

- A RIC scheme applies in $\mathbb{R}^d$, too, but one needs to solve a $(d-1)$-dimensional LP to handle the update.
- This results in an expected time that is of the form $O(d!n + \exp(d))$.
- [Clarkson (1995)]: $O(d^2 n + \exp(d))$, combined with [Kalai (1992)] and [Matoušek&Sharir&Welzl (1996)]: $O(d^2 n + \exp(\sqrt{d \log d}))$.

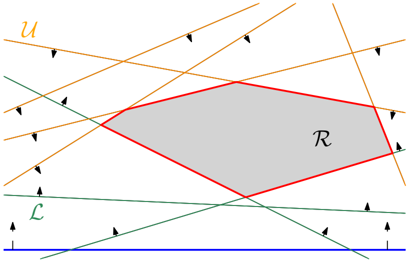
Megiddo's Linear-Time Linear Programming

- Consider an LP for $d = 2$, i.e., in $\mathbb{R}^2$ with two variables x and y, and n constraints.
- Let $\mathcal{R}$ denote the feasibility region. W.l.o.g., we may assume that the LP amounts to seeking a feasible point with maximum y-coordinate: We seek x' such that

$$\max\{y : (x', y) \in \mathcal{R}\} = \max\{y : (x, y) \in \mathcal{R}\}.$$

- Let $\mathcal{U}$ be the set of "upper" constraints that bound $\mathcal{R}$ from above, and let $\mathcal{L}$ be the set of "lower" constraints that bound $\mathcal{R}$ from below.
- The basic idea is to compute the intersection of a line $x = \bar{x}$ with $\mathcal{R}$ in linear time, for some $\bar{x} \in \mathbb{R}$, and to decide whether $x' = \bar{x}$ or $x' < \bar{x}$ or $x' > \bar{x}$.

- Each such decision allows to transform the LP into an equivalent LP, with the same optimum but only 75% of the original constraints.
- Thus, the number of constraints is reduced from n to $^3/_4 n$, $(^3/_4)^2 n$, ...
- An LP with a constant number of constraints is solved by brute force.

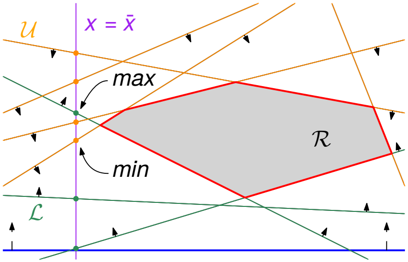


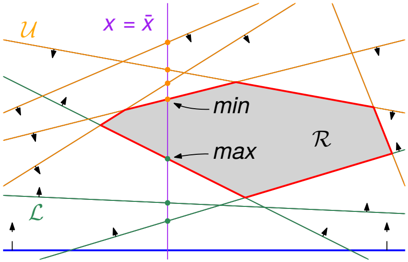
Megiddo's Linear-Time Linear Programming

Lemma 189

One can decide in $O(n)$ time whether the line $x = \bar{x}$ intersects $\mathcal{R}$, for every $\bar{x} \in \mathbb{R}$.

Proof: Intersect $x = \bar{x}$ with all lines of $\mathcal{L}$, and let *max* denote the y-coordinate of the highest intersection with all lines of $\mathcal{L}$. Similar for *min* as the y-coordinate of the lowest intersection with $\mathcal{U}$.
If $max \leq min$ then $\mathcal{R}$ is not empty and $x = \bar{x}$ intersects $\mathcal{R}$. If $max > min$ then $x = \bar{x}$ does not intersect $\mathcal{R}$, or $\mathcal{R}$ is empty. □



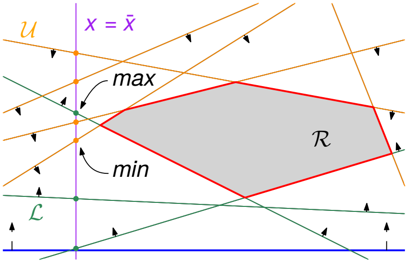


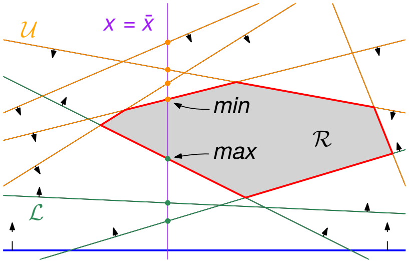
Megiddo's Linear-Time Linear Programming

Lemma 190

1. If the line $x = \bar{x}$ intersects $\mathcal{R}$, then one can decide in $O(n)$ time whether $x' = \bar{x}$ or $x' < \bar{x}$ or $x' > \bar{x}$.
2. If the line $x = \bar{x}$ does not intersect $\mathcal{R}$, then one can decide in $O(n)$ time whether a potentially non-empty $\mathcal{R}$ has to lie to the left or to the right of $x = \bar{x}$. If this decision is not possible then $\mathcal{R}$ is guaranteed to be empty.

Sketch of Proof: This can be decided by inspecting the inclinations of the constraints of $\mathcal{L}$ and $\mathcal{U}$ that determine *min* and *max*. □



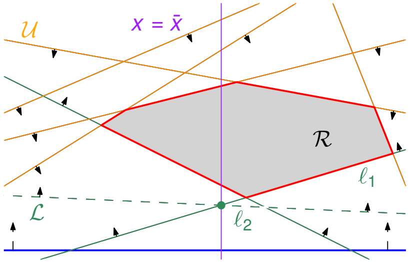


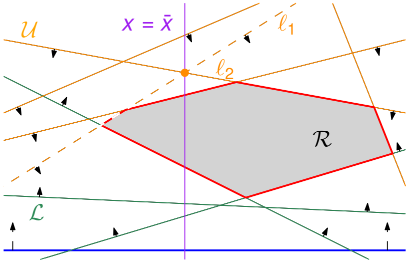
Megiddo's Linear-Time Linear Programming

Lemma 191

Let $\bar{x}$ be the x-coordinate of an intersection point of two constraints ℓ_1, ℓ_2 of $\mathcal{U}$. If $\bar{x} \neq x'$ then we can drop either ℓ_1 or ℓ_2 from $\mathcal{U}$ and derive $\mathcal{U}'$ from $\mathcal{U}$, with $\mathcal{U}' \subset \mathcal{U}$, such that the optimum solution of the LP remains unchanged. This process can be carried out in linear time. Same for an intersection between two constraints of $\mathcal{L}$.

Sketch of Proof: Suppose that $x = \bar{x}$ intersects $\mathcal{R}$ and that $\bar{x} \neq x'$. By Lem. 190, we can decide in $O(n)$ time whether $x' > \bar{x}$ or $x' < \bar{x}$.
W.l.o.g., $x' > \bar{x}$. If ℓ_1 runs above ℓ_2 for all $x > \bar{x}$ then we can drop ℓ_1. Otherwise we can drop ℓ_2. Same for an intersection between two constraints of $\mathcal{L}$. □





Megiddo's Linear-Time Linear Programming

Theorem 192 (*Megiddo (1983,1984)*)

> A linear program with n constraints and d variables can be solved in $O(n)$ time when d is fixed.

Sketch of Proof for $d := 2$:

1. Partition the n_U constraints of $\mathcal{U}$ (arbitrarily) into $\lfloor n_U/2 \rfloor$ pairs. Same for the n_L constraints of $\mathcal{L}$. (Of course, $n_U + n_L = n$.)
2. Compute $\lfloor n_U/2 \rfloor + \lfloor n_L/2 \rfloor$ intersection points among these pairs.
3. Choose the intersection point $(\bar{x}, y)$ whose x-coordinate $\bar{x}$ is the median of all x-coordinates of the intersection points.
4. Use Lem. 191 to discard roughly one quarter of the constraints and recurse on the remaining roughly $\frac{3n}{4}$ constraints.
5. Solve the LP by brute-force means for a constant number of constraints.

- Let $T(n)$ denote the worst-case time to solve an LP with n constraints.
- We get $T(n) = T\left(\frac{3n}{4}\right) + O(n)$, and the Master Theorem 32 implies $T \in O(n)$. □

- Worst-case optimal but slow in practice due to large constant 2^{2^d} hidden in the O-term. For $d := 2, 3$ another (slow) linear-time solution is due to [Dyer (1984)].
- [Seidel (1991)]: Simple randomized LP algorithm with expected time $O(d! \cdot n)$.

Integer Linear Program

Definition 193

An *integer linear program* (ILP) in d variables $x_1, x_2, \ldots, x_d \in \mathbb{R}$ is a linear program with the additional constraint "x_i is integer" for some or all $i \in \{1, 2, \ldots, d\}$.

Solving an ILP: LP relaxation [Agmon (1954)]

- Drop the integer constraints and solve corresponding LP, using the same objective function and all other constraints. E.g., $x_i \in \{0, 1\}$ becomes $x_i \in \mathbb{R}$ with $0 \leq x_i \leq 1$.
- If we are lucky then the LP is "naturally integer" and will return an integer solution.
- Otherwise:
  - Try to establish an integrality gap; i.e., analyze how much rounding increased the cost.
  - Apply branch&bound (aka tree search) or branch&cut.
  - ...

- Note: Rounding a real LP solution to an integer solution may yield a solution that is not feasible or far away from the true optimum!
- Basic practical problem: Even if the LP is solved efficiently, the subsequent transformation of the solution to make it fit the underlying ILP may be costly — it may consume exponential time!

Integer Linear Program

Standard applications of ILP

- The variables represent quantities for which fractions are meaningless, such as the number of workers or the number of busses.
- The variables represent decisions and, thus, should only take on the binary values 0 or 1.

Theorem 194

Integer linear programming is $\mathcal{NP}$-hard.

Sketch of Proof : If we could solve ILP in polynomial time then several $\mathcal{NP}$-hard problems could be solved in polynomial time. E.g., KNAP $\leq_p$ ILP. □

- One can also prove that the decision version of ILP belongs to the class $\mathcal{NP}$. (But this requires some delicate arguments that a polynomial number of digits suffice.)
- In particular, the special case of 0-1 integer linear programming, in which all variables are binary, and only the restrictions must be satisfied, is one of Karp's original 21 $\mathcal{NP}$-complete problems [Karp (1972)].

Circuit Value Problem

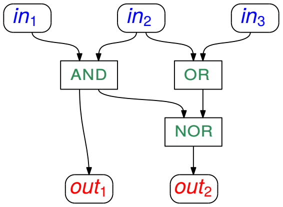
Definition 195 (*Boolean circuit, Dt.: Schaltkreis*)

A *Boolean circuit* with *n* inputs and *m* outputs, for $m, n \in \mathbb{N}$, is a DAG of gates of the following types:

Input gates: The *n* input gates have in-degree zero; their value is `true` or `false`.

Logic gates: The NOT gates have in-degree 1, while AND, OR, NAND, and NOR gates have in-degree 2. All gates follow the laws of Boolean logic. No gate has out-degree zero.

Output gates: Exactly *m* gates are output gates connected to output nodes.



Problem: CIRCUITVALUEPROBLEM (CVP)

Input: A Boolean circuit with *n* inputs and *m* outputs, for $m, n \in \mathbb{N}$.

Output: The output of the Boolean circuit for a given input.

- The BOOLEANFORMULAVALUEPROBLEM is the special case of CVP when the circuit is a tree.

Circuit Value Problem as LP

Theorem 196

CVP is $\mathcal{P}$-complete.

Theorem 197

(The decision version of) LP is $\mathcal{P}$-complete.

Sketch of Proof: One can reduce CVP to LP by creating a variable x_g for each gate g, with the basic constraints $0 \leq x_g \leq 1$.
In addition we introduce the following constraints for the individual gates. E.g.:
Input gate g: $x_g = 1$ for `true` and $x_g = 0$ for `false`.
NOT gate g with $g \equiv \neg a$: $x_g = 1 - x_a$.
AND gate g with $g \equiv a \wedge b$: $x_g \leq x_a$ and $x_g \leq x_b$ and $x_g \geq x_a + x_b - 1$.
OR gate g with $g \equiv a \vee b$: $x_g \geq x_a$ and $x_g \geq x_b$ and $x_g \leq x_a + x_b$.
Easy to see: These constraints force all the gate variables to assume the correct values — 0 for `false` and 1 for `true` — and we can read off the circuit values at the variables of the output gates. (No need to maximize or minimize anything.) □

Knapsack as ILP

Problem: KNAPSACK (KNAP)

Input: A knapsack of capacity $c \in \mathbb{N}$ and n items with sizes $s_1, s_2, \dots, s_n$ and "profits" $p_1, p_2, \dots, p_n$.

Output: A subset I of (the index set of) the objects that fits into the knapsack and maximizes the profit $\sum_{i \in I} p_i$.

- Solution as ILP: We use indicator variables $x_i \in \{0, 1\}$ for all $i \in \{1, 2, \dots, n\}$, with $x_i = 1$ meaning that item i is to be put into the knapsack.

$$\begin{array}{lrcll} \text{maximize:} & \sum_{i=1}^{n} p_i \cdot x_i & & & \\ \text{subject to:} & \sum_{i=1}^{n} s_i \cdot x_i & \leq & c & \\ & x_i & \in & \mathbb{Z} & \text{for all } i \in \{1, 2, \dots, d\} \\ & x_i & \geq & 0 & \text{for all } i \in \{1, 2, \dots, d\} \\ & x_i & \leq & 1 & \text{for all } i \in \{1, 2, \dots, d\} \end{array}$$

3-SAT-CNF as ILP

Problem: 3-Sat-CNF

Input: A propositional formula *A* which is in conjunctive normal form such that every clause consists of exactly (or at most) three literals

Decide: Is *A* satisfiable?

- Solution as ILP: Let $z_1, z_2, \ldots, z_n$ be the Boolean variables. We use indicator variables $x_i \in \{0, 1\}$ for all $i \in \{1, 2, \ldots, n\}$, with $x_i = 1$ if and only if z_i is true.
- Modeling of the clauses as constraints (for $1 \leq i < j < k \leq n$):

$$\begin{aligned}
z_i \vee z_j \vee z_k &\iff x_i + x_j + x_k \geq 1 \\
\bar{z}_i \vee z_j \vee \bar{z}_k &\iff (1 - x_i) + x_j + (1 - x_k) \geq 1 \\
\bar{z}_i \vee \bar{z}_j \vee \bar{z}_k &\iff (1 - x_i) + (1 - x_j) + (1 - x_k) \geq 1 \\
&\vdots
\end{aligned}$$

- Objective function: As for many decision problems, we do not have a genuine objective function — we are only interested in finding a feasible solution. We can, however, maximize 1. Or maximize $x_1 + x_2 + \ldots + x_n$.

INDEPENDENTSET as ILP

Problem: INDEPENDENTSET (IS)

Input: An undirected graph $\mathcal{G} = (V, E)$.

Output: A maximum independent set $I \subseteq V$. (A subset I of V forms an independent set of $\mathcal{G}$ if no pair of vertices of I is connected by an edge of $\mathcal{G}$.)

- Solution as ILP: We use indicator variables $x_v \in \{0, 1\}$ for all $v \in V$, with $x_v = 1$ meaning that node v is in I.

$$\begin{array}{lrcll} \text{maximize:} & \sum_{v \in V} x_v & & & \\ \text{subject to:} & x_v + x_w & \leq & 1 & \text{for all } (v, w) \in E \\ & x_v & \geq & 0 & \text{for all } v \in V \\ & x_v & \leq & 1 & \text{for all } v \in V \end{array}$$

MaximumMatching as ILP

Problem: MaximumMatching

Input: An undirected graph $\mathcal{G} = (V, E)$.

Output: A maximum set of edges $I \subseteq E$ such that no two edges of I share the same node of V.

- Solution as ILP: We use indicator variables $x_e \in \{0, 1\}$ for all $e \in E$, with $x_e = 1$ meaning that edge e is in I.

$$\begin{array}{lrcll} \text{maximize:} & \sum_{e \in E} x_e & & & \\ \text{subject to:} & \sum_{e \text{ incident to } v} x_e & \leq & 1 & \text{for all } v \in V \\ & x_e & \geq & 0 & \text{for all } e \in E \\ & x_e & \leq & 1 & \text{for all } e \in E \end{array}$$

- LP relaxation always gives an integer solution if $\mathcal{G}$ is bipartite!

k-Coloring as ILP

Problem: *k*-**Coloring** (*k*-**Col**)

Input: An undirected graph $\mathcal{G} = (V, E)$, and an integer $k \in \mathbb{N}$.

Decide: Does $\mathcal{G}$ admit a coloring that uses at most k colors? (An assignment of colors to all vertices of $\mathcal{G}$ is called a (vertex) coloring if adjacent vertices are assigned different colors.)

- Solution as ILP: We use indicator variables $x_{v,i} \in \{0, 1\}$ for all $v \in V$ and all colors $i \in \{1, 2, \ldots, k\}$, with $x_{v,i} = 1$ meaning that color i is assigned to node v.
- Constraints:

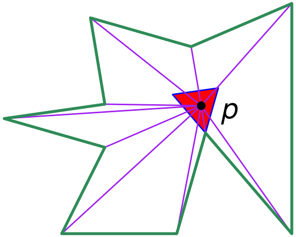
$$\begin{array}{lrcll} \text{maximize:} & & & 1 & \\ \text{subject to:} & \sum_{i=1}^{k} x_{v,i} & = & 1 & \text{for all } v \in V \\ & x_{v,i} + x_{w,i} & \leq & 1 & \text{for all } (v,w) \in E \text{ and all } i \in \{1,2,\ldots,k\} \\ & x_{v,i} & \leq & 1 & \text{for all } v \in V \text{ and all } i \in \{1,2,\ldots,k\} \\ & x_{v,i} & \geq & 0 & \text{for all } v \in V \text{ and all } i \in \{1,2,\ldots,k\} \end{array}$$

- One can also apply ILP to solve Coloring.

Kernel of a Star-Shaped Polygon

Definition 198 (*Star-shaped polygon, Dt.: sternförmiges Polygon*)

A polygonal region P (in the plane) is *star-shaped* if there exists a point $p \in P$ such that for every point $q \in P$ the line segment $\overline{pq}$ lies entirely within P. The set of all points p with this property is called the *kernel* (Dt.: Kern, Nucleus) of P.



- Hence, P is star-shaped if p can "see" every point on the boundary of P.
- Every convex polygonal region is star-shaped.

Lemma 199

The kernel of P is not empty, and P is star-shaped, if and only if the intersection of the "interior" half-planes induced by all oriented edges of the boundary polygon of P is not empty.

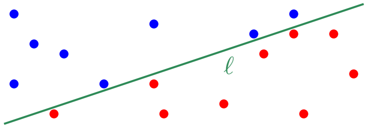
- Formulating the problem as an LP allows to test in linear time whether P is star-shaped. Furthermore, in linear time we can determine a suitable point p if the kernel of P is not empty.

Red-Blue Separation

Problem: **RedBlueSeparation**

Input: A set R of red points and a set B of blue points.

Output: A line ℓ such that all the red points are on one side of ℓ and all the blue points are on the other side, if it exists.



- All possible lines ℓ have the equation $a \cdot x + b \cdot y = c$, for unknown $a, b, c \in \mathbb{R}$.
- If $c \neq 0$ then $a \cdot x + b \cdot y = 1$ with $a, b \in \mathbb{R}$. Otherwise $a \cdot x + b \cdot y = 0$.
- Resulting LP, with $c := 0$ or $c := 1$:

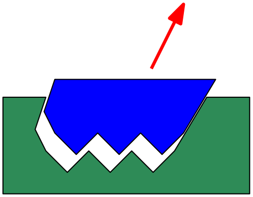
$$\begin{array}{lrcll} \text{maximize:} & 1 & & & \\ \text{subject to:} & a \cdot x_i + b \cdot y_i & \leq & c & \text{for all } (x_i, y_i) \in R \\ & a \cdot x_i + b \cdot y_i & \geq & c & \text{for all } (x_i, y_i) \in B \end{array}$$

- Hence, RedBlueSeparation can be solved in time $O(|R| + |B|)$.

Removal from Mold

Casting (Dt.: Gießen)

- A mold is a 3D shape that forms a hollow cavity.
- Liquid metal is poured into the mold (Dt.: Gussform, Kokille), and one uses gravity (or pressure) to fill the mold.
- Once the metal has solidified, the object cast is removed.
- Permanent mold casting employs reusable molds, which requires the object to be removable from the mold without destroying the mold (or the object).



- Obvious problem: Not all objects are removable from the mold.
- Can we decide efficiently whether an object can be manufactured by casting and, if so, can we find a suitable orientation of the mold and a removal direction?
- We assume that the object to be cast is formed by a polyhedron, i.e., that it is bounded by planar facets.

Removal from Mold

Problem: MOLDREMOVAL

Input: A polyhedral object *P*, with designated (horizontal) top facet, and its corresponding mold.

Output: A direction vector $d \in \mathbb{R}^3$, if it exists, such that *P* can be translated to infinity in direction *d* without intersecting the mold.

- A facet of *P* is called *ordinary facet* if it is not the top facet of *P*.

Lemma 200

The polyhedron *P* can be removed from its mold by a translation in direction *d* if and only if *d* forms an angle of at least 90° with the outward normals of all ordinary facets of *P*.

Lemma 201

The direction vector $d := (d_x, d_y, d_z)$ forms an angle of at least 90° with an outward normal vector $v := (v_x, v_y, v_z)$ if and only if

$$\langle d, v \rangle := d_x \cdot v_x + d_y \cdot v_y + d_z \cdot v_z \leq 0.$$

Removal from Mold

Lemma 202

MoldRemoval can be solved in $O(n)$ time for a polyhedron P with n ordinary facets.

Proof : Since the direction vector d must have a non-zero z-coordinate, we can write d as $(d_x, d_y, 1)$.
Let $v_i := (v_x^i, v_y^i, v_z^i)$ be the outward normal vector of the i-th ordinary facet of P, for $i \in \{1, 2, \ldots, n\}$. Then we get the following simple LP:

$$\begin{array}{ll} \text{minimize:} & d_x + d_y \qquad \text{(or simply 1)} \\ \text{subject to:} & v_x^1 \cdot d_x + v_y^1 \cdot d_y + v_z^1 \leq 0 \\ & v_x^2 \cdot d_x + v_y^2 \cdot d_y + v_z^2 \leq 0 \\ & \vdots \\ & v_x^n \cdot d_x + v_y^n \cdot d_y + v_z^n \leq 0 \end{array}$$

A removal direction d for separating the polyhedron from its mold exists if and only if this LP is feasible, which can be solved in $O(n)$ time. □

Test for Roundness

- A circular annulus (in $\mathbb{R}^2$) is the region between two concentric circles. It is determined by a center $c := (c_x, c_y)$ and two radii, r and R, with $0 \leq r \leq R$.

Problem: MinimumAreaAnnulus

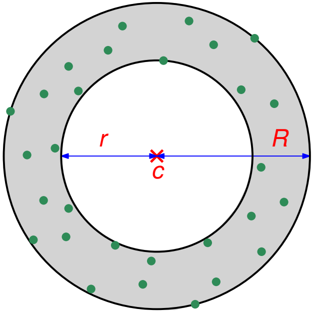
Input: A set S of points in $\mathbb{R}^2$.

Output: A minimum-area circular annulus that contains all points of S.

- MinimumAreaAnnulus can be used to check the "roundness" of a 2D shape by determining the cocircularity of points probed on the shape.
- Hence, we seek to solve the following optimization problem:

$$\begin{array}{ll} \text{minimize:} & \pi(R^2 - r^2) \\ \text{subject to:} & r \leq \|c - p\| \leq R \quad \text{for all } p \in S \end{array}$$

- This does not look like a linear problem, does it?



Test for Roundness as LP

- We introduce two new variables $u, v \in \mathbb{R}$ and a new constraint:

$$u := r^2 - \|c\|^2 \qquad \text{and} \qquad v := R^2 - \|c\|^2 \qquad \text{and} \qquad v \geq u$$

- This transforms the objective function into $\pi(v-u)$, or simply into $v-u$.
- We can re-write the constraints as $r^2 \leq \|c-p\|^2 \leq R^2$.
- Since $\|c-p\|^2 = \|c\|^2 - 2\langle c,p\rangle + \|p\|^2$ for all $p \in S$, we have

$$r^2 \leq \|c-p\|^2 \iff r^2 \leq \|c\|^2 - 2\langle c,p\rangle + \|p\|^2 \iff u + 2\langle c,p\rangle \leq \|p\|^2.$$

- Similarly,

$$\|c-p\|^2 \leq R^2 \iff v + 2\langle c,p\rangle \geq \|p\|^2.$$

- This transforms the objective function and the constraints into a linear program in u, v, c_x, c_y, with the new constraint $v \geq u$.
- We can use $r^2 = u + \|c\|^2$ and $R^2 = v + \|c\|^2$ to reconstruct r and R.
- It cannot happen that r^2 turns out to be negative in an optimum solution: Since we only demand $r^2 \leq \|c-p\|^2$ for all $p \in S$, we could definitely push r^2 to at least 0 by increasing u, while also making the objective $v-u$ smaller!

The End!

I hope that you enjoyed this course, and I wish you all the best for your future studies.

UNIVERSITÄT SALZBURG
Computational Geometry and Applications Lab