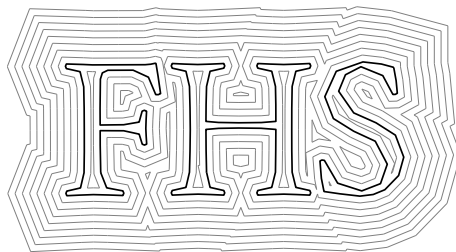


# Numerics and industrial algorithms

Stefan Huber

Dpt. for Information Technologies and Digitalisation  
Salzburg University of Applied Sciences

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# Introduction

**A philosophical introduction.** Computer science and mathematics both belong to the structural sciences. The structural sciences investigate formal systems and abstract structures, like sets, functions, mathematical spaces, algorithms, programs, databases, software architectures and the like. On the other hand, physics or chemistry are natural sciences. They investigate phenomena that we observe in our reality.<sup>1</sup>

The typical subfields of mathematics used in computer science are discrete, like graphs, abstract algebra, number theory and the like. The typical subfields of mathematics used in physics – at least for the purpose of engineering – are continuous, like the Euclidean geometry in  $\mathbb{R}^3$  or differential equations, which describing phenomena in mechanics, electromagnetism, thermodynamics and so on. This is why we tend to find integers in computer science but real numbers in physics.

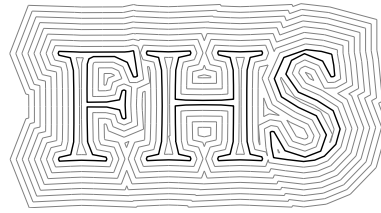
This course is about selected topics that arise from the application of computer science to a continuous mathematical world, as they arise when we deal with problems of the natural sciences, in particular in physics, and engineering. More precisely, this course is about computer science applied to the disciplines of linear algebra, calculus, geometry and topology. When we apply computer science to the real, continuous world, in some sense, we leave the “natural habitat” of computer science. Operations on integers are performed in an exact manner – without numerical loss – by a (digital) computer, but dealing with real numbers is fundamentally impossible for a computer.<sup>2</sup> We are left with approximations of real numbers and each operation introduces loss of precision. The field of numerical analysis investigates the challenges that arise from this fact.

The figure at the title page of these lecture notes exemplifies the type of problems we discuss here. It has been computed by STALGO, a software package to compute so-called straight skeletons.<sup>3</sup> We are given a shape forming the letters “FHS”. Suppose we want to mill out the interior or exterior with a CNC milling machine. In order to do so, we have to compute tool paths for the machine.

<sup>1</sup>The natural sciences use mathematics for modeling and as a language on one hand and as a tool to draw conclusions and extrapolations on the other hand. The classical engineering sciences sit on top of the natural sciences and leverage insights on our real world for technical mechanisms and constructions. Computer science is in some sense different to the classical engineering sciences as it builds upon mathematics directly. Brooks reflects on the nature of programming in his seminal work in the section called “The Joys of the Craft”, when he refers to programming as “slightly removed from pure thought-stuff” and “building castles in the air, from air, creating by exertion of the imagination” [20, p. 7], which highlights the mathematical nature of programming.

<sup>2</sup>There are uncountably many real numbers, but there are only countably many strings over a finite alphabet, so we cannot even represent all possible real numbers even if we would have unlimited memory, like a Turing machine with its infinite memory tape. In particular, there are more real numbers than computer programs or Turing machines. So in this sense we really leave the natural habitat of computer science.

<sup>3</sup><https://www.sthu.org/code/stalgo/>



One strategy is to compute a family of so-called offset curves that are parallel to the shape. But how do we precisely define what an offset curve is?<sup>4</sup> How do we compute them in a computationally efficient and numerically stable way? How do we actually test whether the CNC tool center is currently located within the letter shapes or outside? How can we approximate parts of the tool paths with a smoother representation?

**The organization of these lecture notes.** This course is split into three parts: Numerical programming, numerical mathematics and computational geometry. The first part deals with number representation and numerical analysis. It forms a foundation for numerical computations. The second part is about numerical algorithms within mathematics, in particular linear algebra and calculus.

This first two parts are often summarized by the field called *numerical mathematics*, but since we put some emphasis also on technical details and programming, we instead call the first part *numerical programming*. The following literature is recommended for further reading:

- The lecture notes of Johann Linhart are an excellent and dense compilation on the main topics of numerical mathematics. Johann Linhart was professor at the math department of the University of Salzburg and his lecture notes put an emphasis on the mathematical point of view.  
[18] Johann Linhart. *Numerische Mathematik*. WS 2004/05. URL: [https://www.uni-salzburg.at/fileadmin/multimedia/Mathematik/documents/Num.Mathematik\\_WS2004.pdf](https://www.uni-salzburg.at/fileadmin/multimedia/Mathematik/documents/Num.Mathematik_WS2004.pdf)
- The *Numerical Recipes* belongs to the standard literature of every engineer that produces code and every computer scientist with applications in the real world. This book ships code with a strong emphasis on numerical stability and computational speed. (However, it has not so much emphasis on readable and clean code.)  
[21] William H. Press et al. *Numerical Recipes 3rd Edition: The Art of Scientific Computing*. 3rd ed. New York, NY, USA: Cambridge University Press, 2007. ISBN: 0521880688, 9780521880688
- A comprehensive guide on numerical computation, scientific computing and floating-point arithmetics has been published by Sun microsystems. It contains an article by Goldberg [11] that discusses many details of floating-point units.  
[22] Sun One Studio. *Numerical Computation Guide*. 2003

The field of computational geometry is widely considered of being a part of theoretical computer science, i.e., algorithm theory in the context of geometry. In recent years a development started that expended its scope to also encompass computational topology with major applications in data analysis. The following literature is recommended for further reading:

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<sup>4</sup>If we cannot tell that then we cannot judge whether an algorithm is correct or not. Then we leave the terrain of science.



- This book is largely considered as being the standard book on computational geometry. It contains all classical topics of the field starting in the 1970s.

[4] Mark de Berg et al. *Computational Geometry: Algorithms and Applications*. 3rd ed. Santa Clara, CA, USA: Springer-Verlag TELOS, 2008. ISBN: 3540779736, 9783540779735

- The lecture notes of Martin Held are one of the few that also cover the topics of numerical computation for computational geometry. Martin Held is a professor at the computer science department at the University of Salzburg.

[14] Martin Held. *Computational Geometry*. lecture notes. SS 2018. URL: [https://www.cosy.sbg.ac.at/~held/teaching/compgeo/comp\\_geo.html](https://www.cosy.sbg.ac.at/~held/teaching/compgeo/comp_geo.html)

- The standard book on computational topology is by Herbert Edelsbrunner and John Harer. Herbert Edelsbrunner is a driving figure of both fields, computational geometry and computational topology. He was professor at University of Urbana-Champaign and Duke University and moved 2008 to IST Austria.

[9] Herbert Edelsbrunner and John Harer. *Computational Topology - an Introduction*. American Mathematical Society, 2010. ISBN: 978-0-8218-4925-5

- This is a more recent book that puts more emphasis to discrete geometry.

[7] Satyan L. Devadoss and Joseph O'Rourke. *Discrete and Computational Geometry*. Princeton University Press, 2011. ISBN: 9781400838981



## **Part I**

# **Numerical programming**



# Representation of numbers

A suitable representation of numbers plays an important role when operating with numbers in a computational fashion. The representation of “forty-two” in the decimal system as “42” is by far superior to the roman numeral “XLII” for the execution of arithmetic operations, such as addition and multiplication.

The decimal system’s power allows for the ease at which we operate on numbers and to a certain extent is a key enabler for our modern society, let it be mundane everyday use, science and engineering, finance and business, or politics and administration. The following quote is by Whitehead<sup>1</sup> [24, p. 59]:

By relieving the brain of all unnecessary work, a good notation sets it free to concentrate on more advanced problems, and in effect increases the mental power of the race. Before the introduction of the Arabic notation, multiplication was difficult, and the division even of integers called into play the highest mathematical faculties. Probably nothing in the modern world would have more astonished a Greek mathematician than to learn that, under the influence of compulsory education, a large proportion of the population of Western Europe could perform the operation of division for the largest numbers. This fact would have seemed to him a sheer impossibility. The consequential extension of the notation to decimal fractions was not accomplished till the seventeenth century. Our modern power of easy reckoning with decimal fractions is the almost miraculous result of the gradual discovery of a perfect notation.

## 1.1 The b-adic expansion

### 1.1.1 Mathematical basics

Let us restrict ourselves to non-negative real numbers for now. The representation of forty-two as  $42 = 4 \cdot 10^1 + 2 \cdot 10^0$  allows us to encode this number by the sequence (2, 4) of its digits. We call this a *positional number system*, where the position of a digit determines the value it adds to the number. In this concrete case it is the base-10 positional number system or *decimal system* for short.

Every non-negative real number  $z$  can be represented in the decimal system as a sequence of digits. In a mathematically more precise notation, for each real number  $z \geq 0$  there is a doubly

<sup>1</sup>Whitehead was a mathematician and philosopher. Together with his student Bertrand Russel he wrote the seminal book *Principia Mathematica*.

infinite sequence  $(\dots, a_{-2}, a_{-1}, a_0, a_1, \dots)$  of digits  $a_i \in \{0, \dots, 9\}$ , such that

$$z = \dots + a_1 \cdot 10^1 + a_0 \cdot 10^0 + a_{-1} \cdot 10^{-1} + a_{-2} \cdot 10^{-2} \dots = \sum_{i=-\infty}^{\infty} a_i \cdot 10^i.$$

There is nothing magical about the 10 in the decimal system: The decimal system is just a special case of the *b-adic number expansion*. That is, for every integer  $b > 1$  and every real  $z \geq 0$  there is a doubly infinite sequence  $(a_i)$ , with  $a_i \in \{0, \dots, b-1\}$  called a *digit*, such that

$$z = \sum_{i=-\infty}^{\infty} a_i \cdot b^i. \quad (1.1)$$

For instance, the number  $\pi$  – which is not rational, not even algebraic – would be represented by  $(\dots, 5, 1, 4, 1, 3, 0, 0, 0, \dots)$ , where  $a_0 = 3$  is the digit at position 0.

The number  $b$  is called the *basis* of the *b-adic number expansion*. When calculating with ten fingers then typically the decimal system is easier, for a digital computer with two-valued bits we favor the binary system – the 2-adic expansion –, and for other applications the basis 8 (octal) or the basis 16 (hexadecimal) is more favorable. It is a common notation to write the basis as subindex when there might be confusion. By this notation we have  $11 = 11_{10} = 13_8 = 1011_2 = 14_7$ . When the basis is larger than 10 then we use alphabetical digits  $a, b, c$  and so on, e.g.,  $11 = b_{16}$  or  $24 = 1a_{14}$ .

If there is an index  $m$  such that the digits  $a_i = 0$  for all  $i > m$  then the *b-adic expansion* can be reversed, i.e., for each such sequence there is a non-negative real  $z$  that fulfills eq. (1.1).<sup>2</sup> Moreover, the representation is also unique if there is no index  $k$  such that  $a_i = b-1$  for all  $i < k$ . For instance, in base 10 the real number “one” is both represented as 1.0 by the sequence  $(\dots, 0, 0, 0, 1, 0, \dots)$  and the periodic number  $0.\bar{9}$  represented by  $(\dots, 9, 9, 9, 0, 0, \dots)$ .

### 1.1.2 Finite representations

A real-world computer can only handle a finite number of digits, so we have to restrict the sequence  $(a_i)$  of digits to a finite number of non-zero digits. For instance, the data type `uint32_t` in the programming language C holds only 32 binary digits and is therefore restricted to finitely many digits  $a_0, \dots, a_{31}$ .

**Fixed-point numbers.** In general, however, we could simply choose a fixed, finite number  $m$  of *integral digit* and a finite number  $n$  of *fractional digits* and obtain a so-called *fixed-point number*

$$z = \underbrace{a_{m-1}b^{m-1} + \dots + a_1b^1 + a_0b^0}_{\text{integral part}} + \underbrace{a_{-1}b^{-1} + \dots + a_{-n}b^{-n}}_{\text{fractional part}} = \sum_{i=-n}^{m-1} a_i b^i. \quad (1.2)$$

This fixed-point number is represented by  $m+n$  digits  $a_{m-1}, \dots, a_0, \dots, a_{-n}$ , and all others are zero. That is, the (decimal) point is at a fixed position. For the boundary case  $n = 0$  we have ordinary integers, while for  $n > 0$  we can also represent non-integer numbers. If we choose  $m = 0$  then we obtain numbers in the interval  $[0, 1)$ .

As an example, the number  $\pi$  would be approximated by a fixed-point number to base 10 with  $m = 2$  integral digits and  $n = 5$  fractional digits as

$$\pi \approx 03.14159,$$

---

<sup>2</sup>If there is no such index then the series in eq. (1.1) goes to infinity. However, if there is such an index then there is a smallest such index and we have  $a_m \neq 0$  or the sequence is all zero, i.e.,  $z = 0$ .

where we intentionally also print the leading digit  $a_{m-1} = a_1 = 0$ . Let us denote by  $Q_b^{m,n}$  the set of fixed-point numbers with  $m$  integral and  $n$  fractional digits to the base  $b$ . We can rephrase eq. (1.2) such that

$$z = \left( \sum_{i=0}^{m+n-1} a_{i-n} b^i \right) \cdot b^{-n} \quad (1.3)$$

and therefore  $z = k \cdot b^{-n}$  for some integer  $k$ . From eq. (1.3) we see that a fixed-point number is just a  $(m+n)$ -bit integer scaled by  $b^{-n}$ . Another conclusion we can draw from this point of view is that the set  $Q_b^{m,n}$  has the particular property of being equidistantly distributed on the interval  $[0, b^m)$  with a step size of  $b^{-n}$  between neighboring numbers. We will see that floating-point numbers lack this property.

**Floating-point numbers.** The floating-point number representation extends the fixed-point number representation by the information which index domain  $-n, \dots, m$  is used.

Assume we are given a real number  $z > 0$  and its  $b$ -adic expansion

$$z = a_m b^m + a_{m-1} b^{m-1} + \dots$$

with  $a_m \neq 0$ . That is,  $m$  is the largest index of a non-zero digit  $a_m$ . We obtain  $z'$  from  $z$  by *chopping*<sup>3</sup> to  $p = m - k + 1$  digits by setting

$$z' = \underbrace{a_m b^m + a_{m-1} b^{m-1} + \dots + a_k b^k}_{p \text{ summands}} \approx z. \quad (1.4)$$

We can factor out  $b^{m+1}$  and obtain the so-called *normalized floating-point representation*

$$z' = \underbrace{(a_m b^{-1} + \dots + a_k b^{-p})}_a \cdot b^{m+1} = a \cdot b^{m+1}. \quad (1.5)$$

The number  $a$  is called *mantissa*<sup>4</sup>, the number  $p$  is the *mantissa length* and the number  $m+1$  is the *exponent*. Note that the mantissa is in the interval  $[0, 1)$ . Following these definitions the number  $\pi$  has as normalized floating-point representation to base 10 and chopped to 3 digits

$$\pi \approx 0.314 \cdot 10^1.$$

Its mantissa is 0.314 and its exponent is 1. Note that in eq. (1.5) the number  $m+1$  is not considered fixed but part of the representation along with the mantissa, which allows the decimal point to “float”. (Conversely, the  $n$  in eq. (1.3) is considered to be fixed.)

For technical-didactical reasons we assumed so far that  $z > 0$ , otherwise the index  $m$  in eq. (1.4) may not necessarily exist. However, once we fix  $m$  in eq. (1.5), we can of course set all digits  $a_i = 0$  to represent  $z' = 0$ . Nevertheless, there is no normalized floating-point representation of zero, i.e., we cannot “normalize zero”.

**Distribution of numbers.** In fig. 1.1 we see the distribution of fixed- and floating-point numbers. With loss of generality, we chose two as basis. For reasons of comparison, we use 6 digits to encode the numbers and cover the number range  $[0, 2)$ . For fixed-point numbers we chose 1 integral digit and 5 fractional digits, which leads to an equidistant distribution with a step size

<sup>3</sup>Dt. Abschneiden

<sup>4</sup>Dt. Mantisse

of  $2^{-5} = 0.03125$ . For the floating-point numbers we chose 4 digits for the mantissa and 2 digits for the exponent. We chose the exponent range as  $-2, \dots, 1$ . That is, each interval  $[0, 2^e)$  for  $e \in \{-2, \dots, 1\}$  contains  $2^4 = 16$  equally spaced numbers.

As we can clearly see, floating-point numbers do not possess a “uniform resolution”, but it rather depends on the interval  $[0, 2^e)$  in which a value falls into. This simple fact has profound consequences. For instance, in general we cannot represent the sum of two floating-point numbers in the same representation when we move to a coarser interval. In contrast, fixed-point numbers can be precisely added.<sup>5</sup>

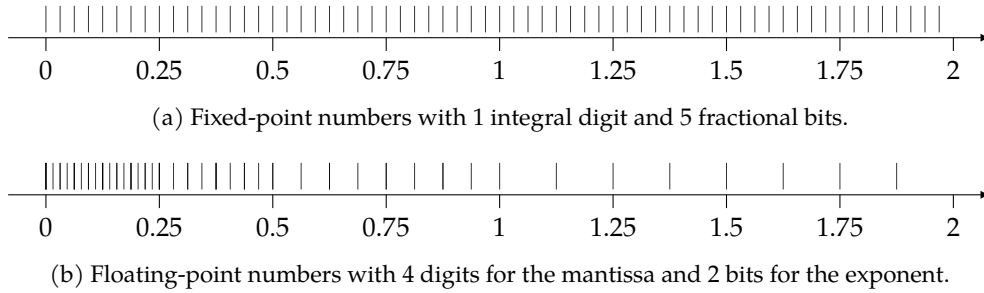


Figure 1.1: Distribution of fixed- and floating-point numbers to cover the range  $[0, 2)$ . In both cases the basis is two and in total 6 digits were used for their representation.

Note that there are  $2^6 = 64$  distinct fixed-point numbers, but only 40 distinct floating-point numbers. For instance, the number zero is represented four times, namely as  $0.0000_2 \cdot 2^k$  for each  $k \in \{-2, 1, 0, 1\}$ . But also the identity  $0.1100_2 \cdot 2^{-1} = 0.0110_2 \cdot 2^0 = 0.0011_2 \cdot 2^1$  leads to multiple representations of the same number; the latter two representations are called *denormalized* – in contrast to *normalized* – since their *most-significant digit*<sup>6</sup> in the mantissa is zero.

If we add one further digit to fixed-point representation as fractional digit then we place between each two neighboring numbers in fig. 1.1a an additional number. The same is true for fig. 1.1b if we add a digit to the mantissa. If, however, we add a digit to the exponent then we can extend the range of the exponent to  $-6, \dots, 1$  and we effectively add 16 numbers for each of the four intervals  $[0, 2^k)$  with  $k \in \{-6, -5, -4, -3\}$ , some of which already being covered. The smallest positive number we can then represent is  $0.0001_2 \cdot 2^{-6} = 2^{-10} = 0.0009765625$ , while in  $Q_2^{1,6}$  the smallest positive number is  $2^{-6} = 0.015625$ .

So the floating-point representation allows us to cover a much larger range in terms of order of magnitude. In other words, on a logarithmic scale, as shown in fig. 1.2, the floating-point numbers are more evenly spaced than fixed-point numbers. Any 32-bit fixed-point number format (like the integers) spans less than 10 decimal orders of magnitude, while a 32-bit floating-point number in IEEE 754 spans 77 decades. The diameter of the observable universe is probably less than  $10^{27}$  m and the Planck length is more than  $10^{-35}$  m, so we could express the entire range of 63 decades with 32-bit floating-point numbers of IEEE 754. Floating-point numbers can even express the wealth of Bill Gates, but 32-bit integers cannot. Any 64-bit fixed-point number format spans about 19 decades, while the 64-bit floating-point numbers of IEEE 754 spans more than 616 decimal orders of magnitude.

<sup>5</sup>The sum may exceed the range covered and cause an overflow, but this issue is of an essentially different nature.

<sup>6</sup>The most-significant digit  $a_i$  is the one with the largest index  $i$ . It has the most influence on the number.



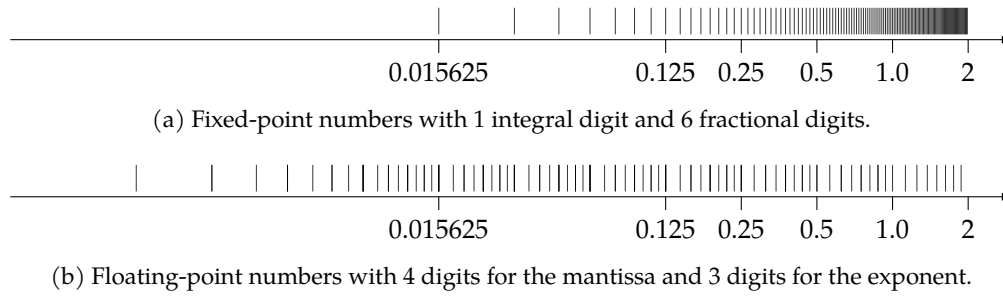


Figure 1.2: Distribution of fixed- and floating-point numbers on a logarithmic scale. In both cases the basis is two and 7 digits were used for their representation.

## 1.2 Hardware number formats

The previous introduction of fixed- and floating-point numbers based on the  $b$ -adic expansion is suitable for mathematical analysis; we will make further use of it in section 2.1. In real-world applications, however, the basis  $b$  is essentially always two<sup>7</sup>, but we also need to deal with negative numbers, which we ignored so far for the sake of simplicity. So let us assume  $b = 2$  as the basis for the remainder of this section and discuss real-world number formats. A digit is therefore called a *bit* (binary digit).

### 1.2.1 Integers

Non-negative integers can directly be treated as fixed-point numbers with  $n = 0$  fractal bits and  $m > 0$  integer bits. So an  $n$ -bit *unsigned integer* with the bits  $a_{n-1}, \dots, a_0$  is an element of  $\mathbb{Q}_2^{n,0}$  and encodes the number

$$z = \sum_{i=0}^{n-1} a_i 2^i. \quad (1.6)$$

By eq. (1.6), the number  $z$  can attain any integer number in the range  $[0, 2^n - 1]$ .

To also accommodate negative integers, one could simply let  $a_{n-1}$  encode the sign, which would give the one's complement format.<sup>8</sup> In this format we would actually distinguish between the encoding of  $+0$  and  $-0$ . We can also ask whether  $(+0) + (-0)$  shall result in  $+0$  or  $-0$  and whether  $(-0) + (+0)$  gives the same result, i.e., whether the operation  $+$  fulfills the commutative property<sup>9</sup>. Arithmetics with one's complement is more complicated.

Instead, the *two's complement*, which has been proposed by John von Neumann, became the dominant format. In two's complement an  $n$ -bit *signed integer* with the bits  $a_{n-1}, \dots, a_0$  encodes

<sup>7</sup>Indeed, the binary coded decimal (BCD) format uses bits to encode numbers, but only to represent decimal digits. That is, the arithmetic is actually based on the decimal system. Legal requirements that financial software must be free of rounding errors essentially implies to do the math in the decimal system. For instance,  $0.1_{10}$  has infinitely many non-zero digits in the 2-adic expansion.

<sup>8</sup>To be precise, in the *one's complement* we negate a number by flipping all bits, so  $-1$  is encoded by all bits set except the least-significant bit.

<sup>9</sup>The commutative property is an essential property and one should think twice sacrificing it. In particular, we do not end up with a so-called *commutative group* anymore from an algebraic point of view. On the other hand, there are other symmetry properties we should consider when defining the operator  $+$ . For instance, how would we argue a tendency towards  $+0$  in the results and break symmetry with  $-0$ ? In a certain sense, we would violate the philosophical principle of Occam's razor, and we should think twice again. By the way, as a personal remark, Occam's razor turned out to be an important design guideline for technical systems.

the number

$$z = -a_{n-1}2^{n-1} + \sum_{i=0}^{n-2} a_i 2^i. \quad (1.7)$$

By eq. (1.7), the number  $z$  can attain any integer number in the range  $[-2^{n-1}, 2^{n-1} - 1]$ .

Figure 1.3 illustrates eq. (1.6) and eq. (1.7). It also illustrates that arithmetic with signed numbers in two's complement is essentially the same as arithmetic with unsigned numbers on a bit level: If we want to add the number 5 to a number then we simply go 5 steps in positive (clockwise) direction. In fig. 1.3 we have 4-bit unsigned and signed integers. In case of signed integers, adding 5 to  $-2$  (encoded as 1110) gives us 3 (encoded as 0011). Likewise, for unsigned integers adding 5 to 14 (encoded as 1110) gives 3 (encoded as 0011) modulo  $2^4$ . This example illustrates a key aspect: On a bit level we executed the same calculation and it can be trivially implemented in hardware.<sup>10</sup>

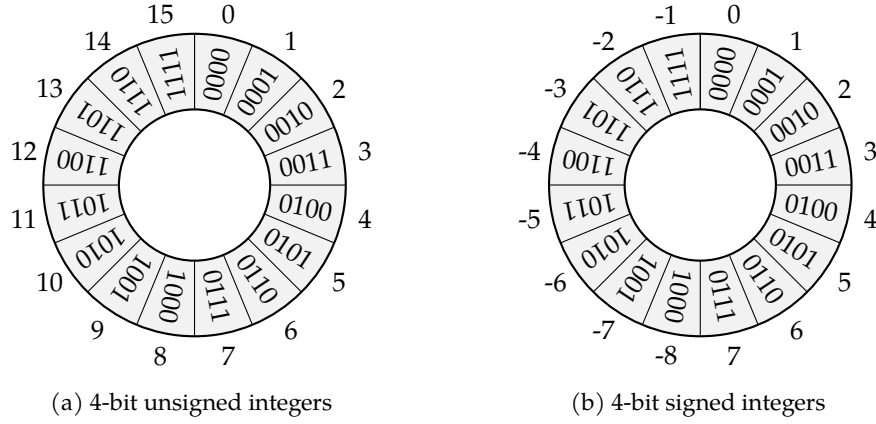


Figure 1.3: Unsigned and signed 4-bit integers. Adding numbers works the same way on a bit level.

### 1.2.2 IEEE 754 floating-point numbers

The prevalent floating-point number format in real-world processors is given by the IEEE 754 standard [1] of the year 1985. The most common binary floating-point data types from this standard are *single precision* (32 bit) and *double precision* (64 bit), but there are others<sup>11</sup>. The binary formats of those two data types are illustrated in fig. 1.4. The mantissa  $a$  is obtained by

$$a = 1.M_2 = 1 + M \cdot 2^{-p},$$

where in “ $1.M_2$ ” we put the mantissa bits  $M$  as fractional part behind “1.”, while in “ $1 + M \cdot 2^{-p}$ ” we see  $M$  as an encoding of an unsigned integer.

This definition differs slightly from  $b$ -adic floating-point numbers: Note that for  $b = 2$  the only non-zero digit is 1. That is, the leading non-zero digit is always 1, so we do not need to explicitly store it. (The attentive reader may have noticed that this argument does not work for

<sup>10</sup>A cascade of  $n$  full adders realizes an  $n$ -bit adder digital circuit.

<sup>11</sup>The Intel x87 floating-point unit also knows a 80 bit format with 64 bits of mantissa. The rise of machine learning in recent years led to the `bf16` format with 8 bits of exponent and 7 bits mantissa.

denormalized numbers.<sup>12)</sup> The real number  $z$ , which is encoded as a binary pattern according to fig. 1.4, is then given by

$$z = (-1)^S \cdot \underbrace{(1 + M \cdot 2^{-p})}_a \cdot 2^{E-B}, \quad (1.8)$$

where  $p$  is the mantissa length (23 for single precision, 52 for double precision) and  $B$  is the so-called *bias* (127 for single, 1023 for double).<sup>13</sup>

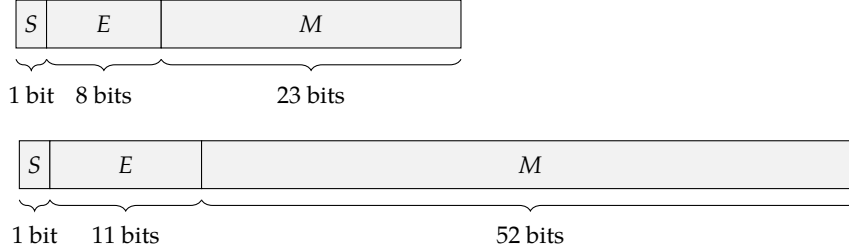


Figure 1.4: The binary layouts of IEEE 754 floating-point numbers with single and double precision. The sign bit is given by  $S$ , the exponent bits by  $E$  and the mantissa bits by  $M$ .

In addition to eq. (1.8) certain binary patterns have a distinguished meaning: A zero is represented by  $E = M = 0$  and we distinguish between  $+0$  and  $-0$  depending on  $S$ .<sup>14</sup> The largest possible exponent, when  $E = 11 \dots 1_2$ , is used to represent  $+\infty$  and  $-\infty$ , but also NaN (not a number).<sup>15</sup> This allows for the following arithmetic laws in IEEE 754:

$$\begin{array}{ll} 1.0 \cdot \pm 0.0 = \pm 0.0 & -1.0 \cdot \pm 0.0 = \mp 0.0 \\ 1.0 \cdot \pm \infty = \pm \infty & -1.0 \cdot \pm \infty = \mp \infty \\ 1.0 \div \pm 0.0 = \pm \infty & -1.0 \div \pm 0.0 = \mp \infty \\ 1.0 \div \pm \infty = \pm 0.0 & -1.0 \div \pm \infty = \mp 0.0 \\ \pm 0.0 \div \pm 0.0 = \text{NaN} & \pm \infty \div \pm \infty = \text{NaN} \\ \pm 0.0 \cdot \pm \infty = \text{NaN} & \end{array}$$

The IEEE 754 standard is extensive and the above presentation gives only a very limited excerpt. In fact, a fully featured implementation of IEEE 754 in a processor is far from being trivial.<sup>16</sup> Goldberg [11] provides many more details regarding programming with IEEE 754 floating-point numbers.

### 1.2.3 Fixed-point formats

Fixed-point numbers typically span a significantly smaller range than floating-point numbers, as we learned in section 1.1.2. However, fixed-point numbers still possess a couple of significant

<sup>12</sup>For  $b$ -adic floating-point numbers we called any representation denormalized, where the most-significant digit of the mantissa was non-zero. In IEEE 754, the *denormalized* numbers are those where  $E = 0$  and  $M \neq 0$ . That is, if  $E = 0$  then we interpret the number as  $0.M_2$ . Handling denormalized numbers can lead to a performance penalty and often we can instruct compilers to be less strict in handling such numbers according the IEEE 754 standard.

<sup>13</sup>The exponent is therefore not encoded by two's complement!

<sup>14</sup>See also the footnote on distinguishing between  $+0$  and  $-0$  for the one's complement on page 11. The IEEE 754 standard defines all these cases.

<sup>15</sup>Actually, different cases of NaN are distinguished.

<sup>16</sup>Processor bugs in the FPU (floating-point unit) are not entirely unusual. The best known example is probably the infamous FDIV bug of early Intel Pentium processors [19]. Also, in the embedded domain some processors only provide a limited feature set of the IEEE 754.

advantages:

Fixed-point arithmetic is exact and arithmetic operations do not introduce numerical errors. This is why fixed-point arithmetic is preferred over floating-point arithmetic in financial software, like in GNU Cash.

IEEE 754-compatible FPUs are hard to implement but fixed-point arithmetic is essentially as simple as integer arithmetic. This makes them favorable for small or cheap embedded processors, signal processors, or dedicated graphics hardware, which may lack a FPU. For instance, the infamous 3D computer game *Doom*<sup>17</sup> used 32 bit signed fixed-point numbers with  $m = 15, n = 16$ , where an increment was  $2^{-16}$ . This allowed Doom to be run on Intel 386 machines.

A typical application in digital signal processing is as follows: An analog-digital converter produces a signal that is further processed, say, by a FIR filter. The domain of the signal is often considered to be in a unit interval, like  $[0, 1]$  or  $[-1, 1]$ . This is why a *digital signal processor* (DSP) often provides native data types and instructions for fixed-point arithmetic.

**Q format.** For binary fixed-point number formats there are a couple of notations to define them. As a reference to the rational numbers  $\mathbb{Q}$ , Texas instruments popularized the so-called Q format:

- $Qm.n$  refers to signed fixed-point numbers with  $m$  integer bits and  $n$  fractional bits.
- $Qn$  refers to the set of signed fixed-point numbers with  $n$  fractional bits and the number  $m$  of integral bits is implicitly given: It is either the number of remaining bits from the register size or is meant to be zero.

Unsigned integers are indicated by prefixing U to Q, so the set of  $UQm.n$  numbers equals the set  $Q_2^{m,n}$ . There is an ambiguity on whether to count the sign bit for signed numbers. One convention says the sign bit is included in  $m$ , so Doom would have used numbers in the format  $Q16.16$ . An alternative convention says that the sign bit is not part of  $m$ , and hence Doom would have used  $Q15.16$ . However, by considering  $m + n$  and comparing with the register size, it is possible to resolve the ambiguity in practice.

If we have a binary representation of a number in  $Qm.n$  or  $UQm.n$  format, as illustrated in fig. 1.5, then we simply read the bit pattern as a signed or unsigned integer and think of it being scaled by  $2^{-n}$ , compare also with eq. (1.3).



Figure 1.5: A number in  $Qm.n$  or  $UQm.n$  format is interpreted as an integer scaled by  $2^{-n}$ .

**Embedded C.** Having fixed-point arithmetic hardware is one thing, but we also require according mechanisms on the software side. For instance, the C programming language knows the data types `float` and `double`, which are the IEEE 754 floating-point number types in single- and double-precision. However, standard C – like C99 or C11 – does not know fixed-point number types and so often vendor-specific C compilers shipped extensions to accommodate fixed-point number types.

Since 2004 there is an ISO/IEC standard, briefly called *Embedded C*, which is based on DSP-C [8]. The current and second version from 2008 is called *ISO/IEC TR 18037:2008* [17]. This

<sup>17</sup>Doom was released in 1993 and constitutes a milestone in games development not only for its 3D graphics.

standard adds fixed-point arithmetic data types and more.<sup>18</sup> The GCC C-compiler supports this standard since 2007 [10]. The Clang compiler of LLVM has some preliminary implementation since 2018 [5]. However, neither fully supports this standard yet.<sup>19</sup>

Embedded C defines two new type specifiers `_Fract` and `_Accum`, which can be used in combination with the type specifiers `short`, `long`, `signed`<sup>20</sup> and `unsigned` and gives rise to the 12 types in table 1.1. The specifier `_Fract` refers to a fixed-point data type with no integral bits, so the number range is within  $[-1, 1)$  for signed types and  $[0, 1)$  for unsigned types. In contrast, `_Accum` also defines integral bits and is, for instance, used when building sums of `_Fract` numbers, i.e., accumulating them. This is why the number of fractional bits of the `_Accum` types match the number of bits of the corresponding `_Fract` types.

In addition, there is a type specifier `_Sat` that makes a type a *saturating* fixed-point type. Adding two large (positive or negative) number of a saturating type does not cause an overflow, as with ordinary integer numbers, but results in the largest (positive or negative) number in the respective number range. This is often the intended behavior in signal processing, e.g., think of mixing audio signals. The header file `stdfix.h` defines `sat`, `fract`, and `accum` as the natural spelling of `_Sat`, `_Fract`, and `_Accum`. The following code listing illustrates the usage of these fixed-point number types:

```
sat fract x = -0.7r;           // Suffix r for fract literals
sat fract y = -0.7r;
printf("x + y = %f\n", (double) (x+y)); // Prints -1.0 due to sat
sat accum a = 0.7k;           // Suffix k for accum literals
sat accum b = 0.7k;
printf("a + b = %f\n", (double) (a+b)); // Prints 1.4 due to accum
```

As usual, the C language does not define the sizes of data types but minimum sizes, which are given in table 1.1. The actual sizes are implementation dependent and may differ between compilers, operating systems or processors. However, there are macros like `FRACT_FBIT`, which gives the number of fractional bits of `_Fract`, or `ULACCUM_IBIT` which gives the number of integral bits of unsigned long `_Accum`.

Type	Suffix	Min.	Type	Suffix	Min.
short <code>_Fract</code>	hr	Q7	short <code>_Accum</code>	hk	Q4.7
<code>_Fract</code>	r	Q15	<code>_Accum</code>	k	Q4.15
long <code>_Fract</code>	lr	Q23	long <code>_Accum</code>	lk	Q4.23
unsigned short <code>_Fract</code>	uhr	UQ7	unsigned short <code>_Accum</code>	uhk	UQ4.7
unsigned <code>_Fract</code>	ur	UQ15	unsigned <code>_Accum</code>	uk	UQ4.15
unsigned long <code>_Fract</code>	ulr	UQ23	unsigned long <code>_Accum</code>	ulk	UQ4.23

Table 1.1: ISO/IEC TR 18027 fixed-point data types with literal suffix and minimum sizes. Here the Q-format does not add the sign bit to the integral bits.

<sup>18</sup>Often, embedded processors follow a Harvard architecture, where program and data memory do not reside in the same address space. Hence, there is a need to specify the address space to which a pointer in C refers to and Embedded C adds support for that.

<sup>19</sup>For instance, clang version 9.0 does not yet support conversion from fixed-point numbers to floating-point numbers or provides the corresponding standard header files. On the other hand, GCC only supports certain targets, for instance x86 is not supported for GCC version 9, but clang does.

<sup>20</sup>As usual for C, `signed` does not need to be explicitly specified.



# Computing with numbers

## 2.1 Floating-point arithmetic

### 2.1.1 Rounding

In order to obtain from a real number  $z$  a floating-point number  $\bar{z}$  with a given mantissa length, we could simply perform the  $b$ -adic expansion and apply chopping. A more accurate result, however, can be obtained if we apply the “usual” rounding: We replace in eq. (1.4) the digit  $a_k$  by  $a_k + 1$  if  $a_{k-1} \geq b/2$ . However, if this results in  $a_k = b$  then we set  $a_k = 0$  and increment  $a_{k+1}$  by one (carry-over), and so forth.

We denote the result by  $\text{rd}_{s,b}(z)$  and call it the *machine number* obtained by rounding to mantissa length  $s$  to the basis  $b$ . For example

$$\text{rd}_{2,10}(0.134) = 0.13 \quad \text{rd}_{2,10}(0.135) = 0.14 \quad \text{rd}_{3,10}(0.1996) = 0.200,$$

where in the last example chopping would have resulted in 0.199, which is less accurate. Among all possible machine numbers of length  $s$  to the basis  $b$  the machine number  $\text{rd}_{s,b}(z)$  is closest to the real number  $z$ . Also note that rounding and chopping yields a rational number from a real number. All machine numbers are rational numbers.<sup>1</sup>

The above method ignores the size of the resulting exponent and the issue of *overflow* for the sake of simplicity. Of course, a real-world implementation of IEEE 754 needs to deal with these cases. If the exponent becomes too small then we could simply set the resulting number to  $+\infty$  or  $-\infty$ . Similarly, if the exponent becomes too large then we can set the resulting number to  $+\infty$  for  $-\infty$ . Besides that IEEE 754 also knows various kinds of rounding modes. The one explained above is known as *round to nearest*,<sup>2</sup> but there are also *round toward 0*, *round toward  $+\infty$* , and *round toward  $-\infty$* . The rounding mode then again influences how overflow is handled.<sup>3</sup>

<sup>1</sup>In addition, IEEE 754 knows special “numbers” like  $+0$ ,  $-0$ ,  $+\infty$ ,  $-\infty$  or NaN.

<sup>2</sup>Actually, IEEE 754 round to nearest applies *round half to even*, where the tie break is not rounding up but rounding to the nearest even integer. So 23.5 and 24.5 are both round to 24. This is also known as the *banker’s rounding*. It reduces the accumulation of rounding errors, whereas tie breaking by rounding up has a bias towards  $+\infty$ .

<sup>3</sup>For instance, if we choose round toward  $-\infty$  or round toward 0 and there is a overflow in positive direction then the result is not  $+\infty$  but the largest finite positive machine number.

### 2.1.2 Error and accuracy

Let  $\tilde{z}$  denote some approximation of the number  $z$ . Then  $|z - \tilde{z}|$  is called the *absolute error* of the approximation and

$$\left| \frac{z - \tilde{z}}{z} \right|$$

is called the *relative error*. Note that the relative error is only defined for  $z \neq 0$ . For instance, let  $\tilde{\pi} = 3.14$  be an approximation of  $\pi = 3.14159 \dots$  then the absolute error is  $0.00159 \dots$  and the relative error is  $\frac{0.00159 \dots}{\pi} \approx 5 \cdot 10^{-4}$ , which is about 0.05 %. Relative errors are often given as percentages when adequate.

If  $\tilde{z}$  was obtained by rounding, i.e.,  $\tilde{z} = \text{rd}_{s,b}(z)$ , then we also speak of an *absolute* resp. *relative rounding error*. For the rounding procedure given in section 2.1.1 the bounds

$$|z - \tilde{z}| \leq \frac{b^k}{2} \quad \text{and} \quad \left| \frac{z - \tilde{z}}{z} \right| \leq \frac{b^{k-m}}{2} = \frac{b^{1-s}}{2},$$

hold, where the latter is only defined for  $z \neq 0$ . The bound for the relative rounding error is also called *relative machine accuracy* or *machine epsilon*. Hence, for IEEE 754 single-precision numbers we obtain a machine accuracy of  $2^{1-24}/2 = 2^{-24} \approx 5.96 \cdot 10^{-8}$  and for double-precision numbers we obtain  $2^{1-53}/2 = 2^{-53} \approx 1.11 \cdot 10^{-16}$ . That is, a single-precision number is accurate for up to about 7 decimal digits and a double-precision number for about 16 decimal digits.<sup>4</sup>

### 2.1.3 Machine operations

Machine operations result in machine numbers. That is, the result of machine operations on machine numbers are rounded in order to again obtain machine numbers. Instead of the usual basic arithmetic operations  $+$ ,  $-$ ,  $\dots$  a processor therefore performs the following machine operations  $\oplus$ ,  $\ominus$ ,  $\odot$ ,  $\oslash$ ,  $\dots$  that involves rounding:

$$\begin{aligned} x \oplus y &= \text{rd}_{s,b}(x + y) \\ x \ominus y &= \text{rd}_{s,b}(x - y) \\ x \odot y &= \text{rd}_{s,b}(x \cdot y) \\ x \oslash y &= \text{rd}_{s,b}(x/y) \end{aligned}$$

Since a change of sign is not influenced by rounding, we could reduce the definition of  $x \ominus y$  to addition, i.e.,  $x \ominus y = \text{rd}_{s,b}(x - y) = \text{rd}_{s,b}(x + (-y)) = x \oplus (-y)$ . That is, the following arithmetic law holds for machine operations:

$$x \ominus y = x \oplus (-y)$$

However, except the above rule, rounding has typically far-reaching consequences such that many usual rules fail to hold! For instance, the order of operations matters because the usual *associative law* does not hold anymore. For example, let  $b = 10$  and  $s = 2$  for  $\text{rd}_{s,b}$  then

$$\begin{aligned} (0.50 \oplus 0.54) \oplus (-0.53) &= 1.0 \oplus (-0.53) = 0.47 \\ 0.50 \oplus (0.54 \oplus (-0.53)) &= 0.50 \oplus 0.01 = 0.51 \end{aligned}$$

<sup>4</sup>The IEEE 754 standard does not define the term *machine accuracy* which unfortunately led to different definitions of this term. Another common definition is: The machine accuracy is  $b^{1-s}$ , which is the difference between 1 and the next larger machine number. This definition leads to a machine accuracy of  $1.19 \cdot 10^{-7}$  resp.  $2.22 \cdot 10^{-16}$  for single resp. double precision. This definition is used for the ISO C standard, Python, Mathematica, MATLAB, or Octavia.



In a Python interpreter we can easily demonstrate this with IEEE 754 floating point numbers as well:

```
>>> e = 2**(-53)
>>> (1.0 + e) + e == 1.0
True
>>> 1.0 + (e + e) == 1.0
False
```

The operations also do not adhere to the distributive law as  $((x \oplus y) \odot z)$  is not necessarily  $(x \odot z) \oplus (y \odot z)$ . Hence, different compilers, different compiler versions, different optimization levels or seemingly trivial changes in the source code<sup>5</sup> can influence the order of machine operations and therefore alter the computational results, even though nothing has changed in a “usual mathematical interpretation” based on real number arithmetic. We need to impute an error corresponding to the machine accuracy to each single operation.

As a consequence the comparison of machine numbers can (virtually) never be done exactly but needs to be performed by means of thresholds.<sup>6</sup> Those so-called *threshold-based* or *epsilon-based comparisons* introduce a fixed application-dependent  $\epsilon > 0$  in order to define the following comparison operators:

$$\begin{aligned} x \dot{=} y &\Leftrightarrow |x - y| \leq \epsilon & x \dot{<} y &\Leftrightarrow x < y \wedge x \dot{\neq} y \\ x \dot{\neq} y &\Leftrightarrow \neg(x \dot{=} y) & x \dot{>} y &\Leftrightarrow x > y \wedge x \dot{\neq} y \\ & & x \dot{\leq} y &\Leftrightarrow x \dot{<} y \vee x \dot{=} y \\ & & x \dot{\geq} y &\Leftrightarrow x \dot{>} y \vee x \dot{=} y \end{aligned}$$

But note that also for these comparison operators many usual laws do not hold anymore. For instance, the *transitive law* fails for  $\dot{=}$  and  $\dot{\leq}$ , e.g., it can be that  $x \dot{=} y$  and  $y \dot{=} z$ , but still  $x \dot{\neq} z$ . Yet, *symmetry* of  $\dot{=}$  and (a weaker form of) *antisymmetry* of  $\dot{\leq}$  do hold, i.e., if  $x \dot{\leq} y$  and  $y \dot{\leq} x$  then  $x \dot{=} y$ .

Finally, it should be mentioned that the arithmetic operations defined in this section do not always correspond to the implementation of some FPUs. For instance, the x87 FPU implements an 80 bit *extended double-precision* floating-point number data type with a 64 bit mantissa. Floating-point operations are done with this 80 bit data type and rounding to a 23 resp. 52 bit mantissa for single or double precision is only done when the result is written into the CPU registers. The later SSE floating-point units of Intel processors do not possess the extended double precision registers anymore and perform operations in single or double precision, which may lead to different results, depending on what FPU unit is utilized by the compiler.

## 2.2 Numerical analysis

### 2.2.1 Numerical algorithms

An *algorithm* transforms input into output in order to solve a specific problem. The problem *sorting* considers a list of numbers<sup>7</sup> as input and asks for a sorted permutation of the list as output. A well known algorithm to the problem *sorting* is for instance *merge sort*. While in algorithm theory we typically ask for the time and space complexity of algorithm, which captures speed and memory footprint, in numerical analysis we also ask for the “numerical quality” of algorithms.

<sup>5</sup>Such as switching from a debug build to a release build.

<sup>6</sup>See also the warning option `-Wfloat-equal` for gcc.

<sup>7</sup>In general a list of elements from a partially ordered set (poset). This not only includes numbers with the ordinary order,  $\geq$ , but for instance also strings with the lexicographical order.

Many problems in the field of numerical mathematics can be phrased as computing a mathematical map that takes a real  $n$ -tuple  $(x_1, \dots, x_n)$  as input and produces a real  $m$ -tuple  $(y_1, \dots, y_m)$  as output. That is, the task is to compute a given function

$$\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^m: x \mapsto \varphi(x),$$

where  $x = (x_1, \dots, x_n)$  is the input tuple and  $\varphi(x)$  is the output tuple. For instance, let us consider the problem of computing the roots of a quadratic polynomial  $az^2 + bz + c$  in the real variable  $z$ . Here the input tuple would be  $(a, b, c) \in \mathbb{R}^3$  and the output tuple would be  $(z_1, z_2) \in \mathbb{R}^2$  of the two roots.<sup>8</sup> A concrete algorithm for this problem could follow the well known formula

$$z_{1,2} = \frac{-b \pm \sqrt{b^2 - 4ac}}{2a}$$

in order to compute the roots. Each of the operations  $+$ ,  $\cdot$ ,  $\sqrt{\phantom{x}}$ ,  $\dots$  we interpret as a computational step in the algorithm, which are composed together to form a map  $\tilde{\varphi}$  that constitutes the algorithm. That is, we could “implement” the above formula by one of many possible sequences of steps, like the following:

$$\begin{pmatrix} a \\ b \\ c \end{pmatrix} \mapsto \begin{pmatrix} -b \\ b^2 \\ ac \\ 2a \end{pmatrix} \mapsto \begin{pmatrix} -b \\ b^2 \\ 4ac \\ 2a \end{pmatrix} \mapsto \begin{pmatrix} -b \\ b^2 - 4ac \\ 2a \end{pmatrix} \mapsto \begin{pmatrix} -b \\ \sqrt{b^2 - 4ac} \\ 2a \end{pmatrix} \mapsto \begin{pmatrix} -b + \sqrt{b^2 - 4ac} \\ 2a \end{pmatrix} \mapsto \begin{pmatrix} -b + \sqrt{b^2 - 4ac} \\ -b - \sqrt{b^2 - 4ac} \\ 2a \end{pmatrix}$$

Some problems  $\varphi$  possess the property that little changes in  $x$  lead to large changes in  $\varphi(x)$ . If the input contains errors – rounding errors, measurement errors, et cetera – and we obtain therefore an approximation  $\tilde{x}$  of the original input  $x$  then this can have large impact on the result. The so-called *condition* of a problem captures this property of a problem. The condition is independent of the specific algorithm but is intrinsic to the problem, it lies in the nature of the specific problem. More precisely, the condition considers the term

$$\|\varphi(\tilde{x}) - \varphi(x)\|,$$

where  $\|\cdot\|$  denotes the norm of a vector.

Let us now consider for a given problem  $\varphi$  an arbitrary algorithm  $\tilde{\varphi}$ . Different algorithms may solve the same problem  $\varphi$  in different ways. The *stability* of an algorithm tells us how sensitive a given algorithm is to changes in the input data. The stability is a property of the algorithm and considers the term

$$\|\tilde{\varphi}(\tilde{x}) - \tilde{\varphi}(x)\|.$$

Some algorithms  $\tilde{\varphi}$  for continuous problems consider certain methods of discretization. For instance in order to differentiate a function  $f: \mathbb{R} \rightarrow \mathbb{R}$  at a position  $x$  we could consider  $(f(x+h) - f(x))/h$ , but of course the result depends on our choice of the *discretization step size*  $h$ . The *consistency* of a numerical algorithm tells us to what extent the algorithm introduces numerical errors independent of errors in the input data. More precisely, the consistency of an algorithm considers the term

$$\|\tilde{\varphi}(x) - \varphi(x)\|.$$

---

<sup>8</sup>We known from calculus that a polynomial of degree two has zero real roots or two (which might be equal). For the sake of simplicity, we assume that roots exist.

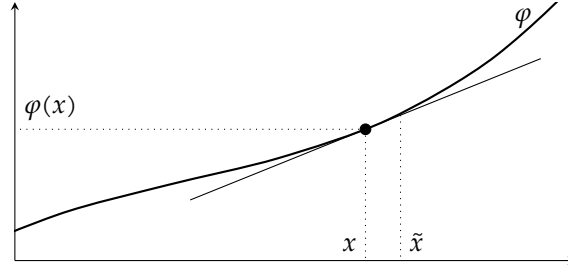


Figure 2.1: The tangent on the function graph of  $\varphi$  at position  $x$  has the slope  $\varphi'(x)$ . At a nearby position  $\tilde{x}$  the function evaluates to  $\varphi(\tilde{x})$ , which can be approximated by the tangent.

### 2.2.2 Condition of a problem

Let us consider a problem  $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^m$ , which takes as input  $x \in \mathbb{R}^n$  and produces an output  $\varphi(x) \in \mathbb{R}^m$  and let us assume that  $\varphi$  can be differentiated.<sup>9</sup>

For the simple case where  $n = m = 1$  we have a function  $\mathbb{R} \rightarrow \mathbb{R}$  and we can consider its function graph, see fig. 2.1. The function  $\varphi$  can be approximated by a linear function at any position  $x \in \mathbb{R}$ . That is, if we consider a  $\tilde{x} \in \mathbb{R}$  close to  $x$  then

$$\varphi(\tilde{x}) \doteq \varphi(x) + \varphi'(x) \cdot (\tilde{x} - x),$$

where  $\doteq$  means that the  $=$  holds only approximately.<sup>10</sup> Similarly, we denote by  $\dot{\leq}$  that  $\leq$  holds only approximately. Then we have

$$\|\varphi(\tilde{x}) - \varphi(x)\| \dot{\leq} \|\varphi'(x)\| \cdot \|\tilde{x} - x\|. \quad (2.1)$$

The above lines were motivated for the case  $n = m = 1$ . However, the beauty of mathematics (or rather the notation) unfolds here in a way such that ineq. (2.1) also holds for  $n, m \geq 1$  if  $\|\varphi'\|$  is suitably interpreted for higher dimensions: Let  $\varphi(x) = (\varphi_1(x), \dots, \varphi_m(x))$  then we denote by  $\varphi'(x)$  the Jacobian matrix

$$\varphi'(x) = \begin{pmatrix} \frac{\partial \varphi_1}{\partial x_1}(x) & \dots & \frac{\partial \varphi_1}{\partial x_n}(x) \\ \vdots & & \vdots \\ \frac{\partial \varphi_m}{\partial x_1}(x) & \dots & \frac{\partial \varphi_m}{\partial x_n}(x) \end{pmatrix}.$$

The Jacobian of  $\varphi: \mathbb{R}^n \rightarrow \mathbb{R}^m$  contains the partial derivatives of all  $m$  elements of  $(\varphi_1(x), \dots, \varphi_m(x))$  by all  $n$  dimensions of  $x = (x_1, \dots, x_n)$ . Hence, it generalizes the tangent slope in fig. 2.1 and if we would have  $n = m = 1$  then the Jacobian is just the ordinary derivative of  $\varphi: \mathbb{R} \rightarrow \mathbb{R}$  at a position  $x$ . Next, for a matrix  $A = (a_{ij})$  we denote by  $\|A\| = \sqrt{\sum_i \sum_j a_{ij}^2}$  the Euclidean matrix norm of  $A$ . (Sometimes it turns out handy to switch to a different  $p$ -norm, but for now we leave

<sup>9</sup>If  $\varphi$  cannot be differentiated at position  $x$  then there is an  $\epsilon > 0$  such that  $\|\varphi(x) - \varphi(\tilde{x})\| > \epsilon$  for some  $\tilde{x} \in [x - \delta, x + \delta]$ , no matter how small  $\delta > 0$  is. That is, we cannot make the output error smaller, no matter how small we make the input error. We will see later that this means that the relative condition is essentially infinite, which means that the problem is in some sense infinitely ill-conditioned.

<sup>10</sup>We can interpret the right-hand side as a Taylor polynomial of degree 1. So the remainder of the Taylor series is in  $O(\|\tilde{x} - x\|^2)$ , i.e., the error of  $\doteq$  converges to zero at order  $\|\tilde{x} - x\|^2$ .

it there.<sup>11)</sup> Hence, the norm of the Jacobian is given by

$$\|\varphi'(x)\| = \sqrt{\sum_{i=1}^n \sum_{j=1}^m \left( \frac{\partial \varphi_j}{\partial x_i}(x) \right)^2}.$$

Using this interpretation for  $\|\varphi'\|$  generalizes ineq. (2.1) to higher dimensions.<sup>12</sup> Note that ineq. (2.1) tells us by how much the output of  $\varphi$  may change at most if we change the input. This immediately motivates the definition of the *absolute condition* of  $\varphi$  by

$$\kappa_{\text{abs}} = \|\varphi'(x)\|$$

and we obtain

$$\|\varphi(\tilde{x}) - \varphi(x)\| \leq \kappa_{\text{abs}} \cdot \|\tilde{x} - x\|.$$

We can rearrange this inequality to

$$\frac{\|\varphi(\tilde{x}) - \varphi(x)\|}{\|\varphi(x)\|} \leq \frac{\|x\|}{\|\varphi(x)\|} \kappa_{\text{abs}} \cdot \frac{\|\tilde{x} - x\|}{\|x\|}.$$

This inequality motivates the definition of the *relative condition* of  $\varphi$  as

$$\kappa_{\text{rel}} = \frac{\|x\|}{\|\varphi(x)\|} \kappa_{\text{abs}}$$

and we obtain

$$\frac{\|\varphi(\tilde{x}) - \varphi(x)\|}{\|\varphi(x)\|} \leq \kappa_{\text{rel}} \cdot \frac{\|\tilde{x} - x\|}{\|x\|}.$$

We call a problem being *ill-conditioned*<sup>13</sup> if  $\kappa_{\text{abs}}$  or  $\kappa_{\text{rel}}$  are significantly greater than 1 and otherwise *well-conditioned*<sup>14</sup>. However, there is no general rule to what “significantly” actually means, so it depends on the specific application at hand.

As a simple example we consider the calculation of square roots, so our problem is given by  $\varphi(x) = \sqrt{x}$ . We obtain  $\kappa_{\text{abs}} = |\varphi'(x)| = |\frac{1}{2\sqrt{x}}|$  and  $\kappa_{\text{rel}} = |\frac{x}{\sqrt{x}} \cdot \frac{1}{2\sqrt{x}}| = \frac{1}{2}$ . The relative condition is unconditionally good, however the absolute condition is bad when  $x$  is close to zero. Also note that the absolute condition, but also the relative condition, is not defined at  $x = 0$ .

**Condition of addition and subtraction.** We would like to determine the condition of the addition resp. subtraction of two real numbers. So we consider  $\varphi: \mathbb{R}^2 \rightarrow \mathbb{R}$  with  $\varphi(x_1, x_2) = x_1 + x_2$ . The partial derivatives of  $\varphi$  with respect to  $x_1$  is 1 and the same holds for  $x_2$ . Hence, by definition

$$\varphi' = \begin{pmatrix} \frac{\partial \varphi}{\partial x_1} & \frac{\partial \varphi}{\partial x_2} \end{pmatrix} = \begin{pmatrix} 1 & 1 \end{pmatrix}.$$

<sup>11</sup>can interpret the set of real  $m \times n$  matrices as a vector space  $V$  of dimension  $m \cdot n$ . In general, for a vector space  $V$  a norm  $\|\cdot\|$  is any map  $V \rightarrow \mathbb{R}$  with the following properties:  $\|x\| \geq 0$ ,  $\|x\| = 0 \Leftrightarrow x = 0$ ,  $\|\lambda x\| = |\lambda| \|x\|$ ,  $\|x + y\| \leq \|x\| + \|y\|$  for all  $\lambda \in \mathbb{R}$  and  $x, y \in V$ . The Euclidean norm is also known as the 2-norm, which is a special case of the  $p$ -norm. For  $V = \mathbb{R}^d$  and  $x = (x_i) \in \mathbb{R}^d$  the  $p$ -norm of  $x$  is defined by  $\|x\|_p = \sqrt[p]{\sum_i |x_i|^p}$ . The 1-norm is also known as sum norm as  $\|x\|_1 = \sum_i |x_i|$  and the  $\infty$ -norm is also known as maximum norm  $\|x\|_\infty$  because  $\lim_{p \rightarrow \infty} \|x\|_p = \max_i |x_i|$ . Likewise, we define the  $p$ -norm of a matrix  $A = (a_{ij})$  as  $\|A\|_p = \sqrt[p]{\sum_{i,j} |a_{ij}|^p}$ .

<sup>12</sup>Actually, for  $n = m = 1$  equality holds in ineq. (2.1). However, for higher dimensions this is not true.

<sup>13</sup>Dt. schlecht konditioniert

<sup>14</sup>Dt. gut konditioniert

The norm of this matrix gives the absolute condition:

$$\kappa_{\text{abs}} = \|\varphi'\| = \sqrt{1^2 + 1^2} = \sqrt{2}.$$

The relative condition<sup>15</sup> is therefore

$$\kappa_{\text{rel}} = \sqrt{2} \cdot \frac{\sqrt{x_1^2 + x_2^2}}{|x_1 + x_2|}.$$

Note that when  $x_1 = -x_2$  then the relative condition is undefined. But even if  $x_1 \approx -x_2$  then  $\kappa_{\text{rel}}$  is becoming very large and hence addition becomes very ill-conditioned. This leads to a very important observation:

Adding two numbers with similar absolute values but different sign – or subtracting two similar numbers – is very ill-conditioned!

This phenomenon is called *cancellation*: When subtracting two similar numbers the digits cancel each other out and in the floating-point representation the remaining digits constitute the remaining significance resp. accuracy.

In the following example we calculate the difference  $\pi - \sqrt[3]{31}$  using 4-digit floating-point to the base 10. We obtain  $\text{rd}_{4,10}(\pi) = 0.3142 \cdot 10^1$  and  $\text{rd}_{4,10}(\sqrt[3]{31}) = 0.3141 \cdot 10^1$  from which we calculate the difference  $0.1 \cdot 10^{-2}$ . The digits 3, 1, 4 canceled each other out. The exact result would have been  $\pi - \sqrt[3]{31} = 0.0212 \dots \cdot 10^{-2}$ . The absolute error is just  $7.88 \dots \cdot 10^{-4}$ . However, the relative error is about 370 %, although the relative rounding errors are no larger than about 0.05 %!

### 2.2.3 Stability of an algorithm

Many numerical algorithms can be described as a sequence of elementary calculation steps. Each step solves an elementary problem  $\psi_1, \dots, \psi_n$  and altogether they solve the original problem  $\varphi$  and hence  $\varphi(x) = \psi_n(\dots \psi_2(\psi_1(x)) \dots)$  or more briefly  $\varphi = \psi_n \circ \dots \circ \psi_1$ . The stability<sup>16</sup> of an algorithm results from the conditions of the individual steps  $\psi_i$ : If one step is ill-conditioned then the entire algorithm – the “chain of steps” – is *instable*.

As an example we consider the problem of solving the quadratic equation  $x^2 + 2px + q = 0$ . We are only interested in the larger of possibly two solutions and we simply assume that a solution actually exists.<sup>17</sup> Hence, our problem  $\varphi: \mathbb{R}^2 \rightarrow \mathbb{R}$  is given by

$$\varphi(p, q) = -p + \sqrt{p^2 - q}.$$

A first algorithm could simply perform the stepwise calculations obtained from the formula above. We then obtain the following sequence of elementary operations:

**procedure** QUADEQUATION( $p, q$ )

$s \leftarrow p^2$

$t \leftarrow s - q$

$u \leftarrow \sqrt{t}$

$\triangleright u \text{ is } \sqrt{p^2 - q}$

<sup>15</sup>If we would have used the 1-norm for the definitions of conditions then we would have  $\kappa_{\text{rel}} = \frac{|x_1| + |x_2|}{|x_1 + x_2|}$ .

<sup>16</sup>In [18] the stability is also called *condition of an algorithm*.

<sup>17</sup>A real solution exists in  $\mathbb{R}$  if  $p^2 \geq q$ .

```

     $r \leftarrow -p + u$ 
    return  $r$ 
end procedure

```

If  $p^2 \gg q$  then  $u \approx \sqrt{p^2} = |p|$ . In other words, if  $p > 0$  and  $p^2 \gg q$  then the fourth step is ill-conditioned because  $p \approx u$  and we suffer cancellation. But there is hope that a different algorithm might perform better.

We may know, or at least easily verify, that the following equality holds:

$$-p + \sqrt{p^2 - q} = \frac{-q}{p + \sqrt{p^2 - q}}.$$

We interpret this equality as a mathematically reformulation of the problem. That is, as a numerical problem as such it is just the same. However, the point is here that the right hand side gives us a hint to a different algorithm – as a sequence of elementary steps – to the same problem:

```

procedure QUADEQUATIONALT( $p, q$ )

```

```

     $s \leftarrow p^2$ 

```

```

     $t \leftarrow s - q$ 

```

```

     $u \leftarrow \sqrt{t}$ 

```

$\triangleright u$  is  $\sqrt{p^2 - q}$

```

     $v \leftarrow p + u$ 

```

```

     $r \leftarrow -q/v$ 

```

```

    return  $r$ 

```

```

end procedure

```

This algorithm is now stable for  $p > 0$ . However, conversely to the first algorithm, it is instable for  $p < 0$  and  $p^2 \gg q$ . So depending on  $p$  and  $q$  we would rather choose the first algorithm or the second algorithm from a numerical analysis point of view.

Nevertheless, both algorithms are instable when  $s \approx q$ , meaning  $p^2 \approx q$ , due to the second step. However, in this case the problem  $\varphi$  has either no solution or the two solutions are very close to each other as the extreme value of the parabolic function graph is close the  $x$ -axis. Hence, little changes in  $p$  or  $q$  have big impacts to the solutions. In other words, our intuition says that the problem is already ill-conditioned for  $p^2 \approx q$ , which we can confirm:

$$\kappa_{\text{abs}} = \|\varphi'(p, q)\| = \left\| \begin{pmatrix} -1 + \frac{p}{\sqrt{p^2 - q}} & \frac{-1}{2\sqrt{p^2 - q}} \end{pmatrix} \right\| \geq \frac{1}{2\sqrt{p^2 - q}}$$

because in general  $\|(x \ y)\| \geq |y|$  for all  $x, y \in \mathbb{R}$ . That is, this mathematical framework tells us that there is no hope in searching for another algorithm that would be numerically stable in this case, because the issue lies within the numerical problem itself, not a particular numerical algorithm.

## **Part II**

# **Numerical mathematics**





# Systems of linear equations

Systems of linear equations play an essential role not only for all technical disciplines, but also in physics, chemistry, economics, and essentially in all fields where mathematics in general plays a role. In computer science alone, we have applications in computer vision, machine learning, computational geometry, and so on. In industrial automation a prime example of systems of linear equations is the forward and backward kinematic in robotics.

## 3.1 Introduction

In the following we consider a system

$$\begin{aligned} a_{11}x_1 + \dots + a_{1n}x_n &= b_1 \\ &\vdots \\ a_{n1}x_1 + \dots + a_{nn}x_n &= b_n \end{aligned}$$

of linear equations with variables  $x_j \in \mathbb{R}$  and real coefficients  $a_{ij} \in \mathbb{R}$  at the left-hand side and constants  $b_i \in \mathbb{R}$  at the right-hand side. Using matrices we can write more concisely

$$A \cdot x = b,$$

and we assume that the real  $n \times n$  matrix  $A = (a_{ij})$  is regular<sup>1</sup>,  $x = (x_1, \dots, x_n)$  and  $b = (b_1, \dots, b_n)$ . Then we know from linear algebra that there is a unique  $x \in \mathbb{R}^n$  such that  $A \cdot x = b$ . Moreover, if we would know the inverse Matrix  $A^{-1}$  of  $A$  already then we could simply calculate  $x = A^{-1} \cdot b$ .

In the following, we will discuss how to solve linear systems, how to compute the inverse  $A^{-1}$  and what we can say in terms of numerical stability. Then we generalize the problem setting to non-regular matrices  $A$ , which leads us to approximation tasks and regression, the principle of least squares and certain matrix factorizations of  $A$ .

## 3.2 Gaussian elimination

### 3.2.1 Right triangular matrix and back substitution

The well known Gaussian elimination is able to solve the system  $A \cdot x = b$ , but can also be used to find the inverse  $A^{-1}$ . The Gaussian elimination method is also known as *row reduction*, which essentially already describes how it works:

<sup>1</sup>Regular means invertible. That is, a matrix  $A^{-1}$  of the same dimension exists such that  $A \cdot A^{-1} = A^{-1} \cdot A = I$ , where  $I$  is the identity matrix. Another common notation is  $I = (\delta_{ij})$ , where  $\delta_{ij}$  denotes the Kronecker-delta, which is 1 when  $i = j$  and 0 otherwise. A square matrix  $A$  is regular iff its determinate  $\det A \neq 0$ .

In a first step we subtract from the  $i$ -th equation the  $a_{i1}/a_{11}$ -multiple of the first equation for all  $2 \leq i \leq n$ . We receive a new  $i$ -th row in the matrix  $A$ :

$$(a_{i1} \ a_{i2} \ a_{i3} \ \dots \ a_{in}) - \frac{a_{i1}}{a_{11}} (a_{11} \ a_{12} \ a_{13} \ \dots \ a_{1n}) = (0 \ a_{i2}^{(1)} \ a_{i3}^{(1)} \ \dots \ a_{in}^{(1)}).$$

By doing so, we do not alter the solution of the original system, yet we introduced leading zeros – hence “row reduction” – to all equations below the first one. So after the first step we have this new equivalent system:

$$\begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ 0 & a_{22}^{(1)} & \dots & a_{2n}^{(1)} \\ 0 & a_{32}^{(1)} & \dots & a_{3n}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & a_{n2}^{(1)} & \dots & a_{nn}^{(1)} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2^{(1)} \\ b_3^{(1)} \\ \vdots \\ b_n^{(1)} \end{pmatrix}, \quad (3.1)$$

where  $a_{ij}^{(1)} = a_{ij} - a_{i1} \cdot a_{1j}/a_{11}$ ,  $b_i^{(1)} = b_i - b_1 \cdot a_{i1}/a_{11}$  for all  $1 \leq i, j \leq n$ . We now repeat this row reduction in a way that we subtract from the  $i$ -th row the  $a_{i2}^{(1)}/a_{22}^{(1)}$ -multiple of the second row for all  $3 \leq i \leq n$ . This introduces leading zeros in the second column of row 3 to  $n$ :

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} & \dots & a_{1n} \\ 0 & a_{22}^{(1)} & a_{23}^{(1)} & \dots & a_{2n}^{(1)} \\ 0 & 0 & a_{32}^{(2)} & \dots & a_{3n}^{(2)} \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & a_{n2}^{(2)} & \dots & a_{nn}^{(2)} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2^{(1)} \\ b_3^{(2)} \\ \vdots \\ b_n^{(2)} \end{pmatrix}. \quad (3.2)$$

We keep doing row reduction and successively eliminate all elements below the diagonal of the matrix. After the  $(n-1)$ -th step we therefore obtain a so-called *right (upper) triangular matrix*, which is typically denoted by the letter  $R$ . Hence, with  $R = (r_{ij})$  we end up with the system

$$\begin{aligned} r_{11} \cdot x_1 + r_{12}x_2 + \dots + r_{1n}x_n &= b'_1 \\ r_{22}x_2 + \dots + r_{2n}x_n &= b'_2 \\ &\vdots \\ r_{nn}x_n &= b'_n, \end{aligned} \quad (3.3)$$

which has a solution space identical to the original system of linear equations. From the last equation we conclude  $x_n = b'_n/r_{nn}$ , and we can *back-substitute*  $x_n$  into the other equations. Now we can determine  $x_{n-1}$  and so forth in order to obtain the solution vector  $(x_1, \dots, x_n)$ . We can summarize the method of Gaussian elimination as follows:

A system of linear equations with a right triangular matrix is easily solved using back-substitution and Gaussian elimination translates the original system into a right triangular matrix form.

### 3.2.2 Pivoting

In the first step of the Gaussian elimination we divided by  $a_{11}$  and in the subsequent steps we divided by  $a_{ss}^{(s-1)}$ . Of course, this only works if these elements are not zero. If this would be the

case then at least one the elements below in the same column must be non-zero<sup>2</sup> and we can simply exchange the two rows in order to make  $a_{ss}^{(s-1)}$  non-zero.

This procedure is called *pivoting* and the element  $a_{ss}^{(s-1)}$  is called the *pivot*. Regarding the numerical condition of the division operation, however, we do not only require  $a_{ss}^{(s-1)} \neq 0$  but we want its absolute value to be as large as possible. The reason for this is that the absolute condition of the operation  $\varphi(x) = a/x$  is

$$\kappa_{\text{abs}} = \frac{|a|}{x^2},$$

which is the smaller the larger  $x$  is. Hence, in the  $s$ -th step we first look for the largest value of  $|a_{ks}^{(s-1)}|$  among  $|a_{ss}^{(s-1)}|, \dots, |a_{ns}^{(s-1)}|$  and then swap the  $s$ -th and  $k$ -th row.

From a numerical point of view we could also swap columns in order to make the pivot even larger. However, then we would need to do bookkeeping on the column transpositions because each of them also swaps elements in the solution vector, which have to be undone at the very end of the Gaussian elimination. We do not go into further details here as Gaussian elimination is anyhow not the first choice in practice.

However, we would like to mention that the Gaussian elimination can also be used with singular coefficient matrices  $A$ . The solution space is then either empty (if the system cannot be solved) or it is an affine-linear subspace of dimension at least zero. When the dimension is zero then the space consists of a single solution.

### 3.2.3 Time complexity

In the  $s$ -th row reduction step we modify  $(n-s)^2$  elements of  $A$  and  $(n-s)$  elements of  $b$ . Each modification involves a constant number of elementary<sup>3</sup> operations. Hence, altogether we have

$$\sum_{s=1}^{n-1} (n-s)^2 + (n-s) = \sum_{s=0}^{n-1} s^2 + s = \underbrace{\frac{(n-1)n(2n-1)}{6}}_{\text{in } A} + \underbrace{\frac{(n-1)n}{2}}_{\text{in } b} \sim \frac{n^3}{3} \quad (3.4)$$

modifications, where  $\sim$  means *asymptotically equivalent*.<sup>4</sup> Hence, in  $O(n^3)$  time we obtain the right triangular form.

The back-substitution of  $x_s$  requires us to modify  $s-1$  entries in the vector  $b$ : We keep modifying  $b$  by plugging in known  $x_s$  in eq. (3.3) on the left-hand side of the equation and subtracting those terms onto  $b$  on the right-hand side. That is, for  $x_n$  we have modify  $n-1$  elements of  $b$ , for  $x_{n-1}$  we modify  $n-2$  elements in  $b$ , and so on. This is repeated until  $b$  is the solution vector. This leads to

$$\sum_{s=2}^n (s-1) = \sum_{s=1}^{n-1} s = \frac{(n-1)n}{2} \sim \frac{n^2}{2} \quad (3.5)$$

element modifications of the vector  $b$  until we have the solution vector  $x$ . Hence, the back-substitution takes  $O(n^2)$  time. Altogether we can solve  $A \cdot x = b$  in  $O(n^3)$  time, which is spent in asymptotically  $n^3/3$  element modifications, as the row-reduction dominates.

<sup>2</sup>Otherwise the  $(s-1)$ -th and the  $(s-2)$ -th column would be linearly dependent and the original matrix  $A$  could not have been regular and  $\det A = 0$ .

<sup>3</sup>An elementary operation – such as add and multiply – can be done in constant time. For instance, a processor has machine instructions to add and multiply elements.

<sup>4</sup>The equivalence relation  $f(n) \sim g(n)$  is defined as  $\lim_{n \rightarrow \infty} f(n)/g(n) = 1$ .

### 3.2.4 Multiple right-hand sides

From the analysis of the time complexity we learned that the back-substitution takes  $O(n^2)$  time, while the row reduction itself takes  $O(n^3)$  time. In some sense, we could perform the back-substitution a linear number of times without compromising the overall time complexity of  $O(n^3)$ . In particular, we could consider  $n$  right-hand sides  $b_1, \dots, b_n$  and solve all the systems  $A \cdot x = b_i$ .

Let us therefore consider  $r$  right-hand sides  $b_1, \dots, b_r$  and join them column-wise to a matrix  $B = (b_1, \dots, b_r)$ . We then look for a  $n \times r$  matrix  $X$  that solves

$$A \cdot X = B.$$

The row reduction and the back-substitution work the same way, we just have to modify all  $r$  columns of  $B$  instead of a single column vector  $b$ . Following eq. (3.4) and eq. (3.5) we therefore have asymptotically

$$\frac{n^3}{3} + r \frac{n^2}{2} + r \frac{n^2}{2} = \frac{n^3}{3} + rn^2 \quad (3.6)$$

element modifications until we obtain the solution matrix  $X$ . Hence, solving  $r \in O(n)$  linear systems with the same coefficient matrix  $A$  costs the same as solving a single system in terms of the  $O$ -notation, namely  $O(n^3)$  time.

**Inverse of a matrix.** For the special case where  $B$  is the identity matrix we obtain a matrix  $X$  such that  $A \cdot X = I$ . This is just the definition of the inverse matrix  $A^{-1}$  of  $A$ . The Gaussian elimination can therefore be used to compute the matrix inverse and it requires asymptotically

$$\frac{4}{3}n^3$$

element modifications, which is in  $O(n^3)$ , by eq. (3.6). If we look more closely, we can exploit the fact that  $B$  contains mostly zeros, which allows for improvements to reduce the number of operations, but it does not improve the  $O(n^3)$  bound. See [21] for details.

## 3.3 Linear regression

### 3.3.1 Overdetermined system of equations

In the introduction to this chapter we started with a system of linear equations  $A \cdot x = b$ , where the square matrix  $A$  was regular. In other words, we had exactly as many equations as variables and the rank of  $A$  was maximal, i.e., the rows of  $A$  were linearly independent.

In this section we study an *overdetermined* system of linear equations, which possesses more equations than variables. That is, we consider a system  $A \cdot x = b$  of  $m$  equations in  $n$  variables, where  $m > n$  and  $A$  is therefore an  $m \times n$  matrix. Such a system cannot be solved exactly in general, which means that there is no  $x \in \mathbb{R}^n$  such that  $A \cdot x = b$ .

However, we can ask which  $x \in \mathbb{R}^n$  minimizes the error  $\|A \cdot x - b\|$ . Minimizing  $\|A \cdot x - b\|$  is equivalent to minimizing  $\|A \cdot x - b\|^2$ , hence this problem can be rephrased into finding  $x \in \mathbb{R}^n$  such that

$$\sum_{i=1}^m (a_{i1}x_1 + \dots + a_{in}x_n - b_i)^2$$

is minimized. This leads to the method of *least squares*, which dates back to Carl Friedrich Gauss. First applications of least squares were in geodesy and astronomy.<sup>5</sup> Least squares are a standard tool in regression analysis, they are a fundamental tool in data fitting<sup>6</sup> and often are used as an introduction into machine learning of linear models.

### 3.3.2 Normal equations

We are given a real  $m \times n$ -matrix  $A$  and a vector  $b \in \mathbb{R}^m$  and we seek for a  $x \in \mathbb{R}^n$  that minimizes  $\|A \cdot x - b\|$ . The term  $A \cdot x$  expresses the transformation of a point  $x \in \mathbb{R}^n$  into a point  $A \cdot x \in \mathbb{R}^m$  and the set of all such transformed points form  $\text{im } A$ , the image of  $A$ :

$$\text{im } A = \{Ax : x \in \mathbb{R}^n\}.$$

Note that  $\text{im } A$  lives in  $\mathbb{R}^m$ , and from linear algebra we know that it forms in fact a linear subspace<sup>7</sup> of  $\mathbb{R}^m$ . So our goal is now to find a point in  $\text{im } A$  that is closest to  $b$ . In case that  $b \in \text{im } A$  then  $A \cdot x = b$  can be solved exactly. In the general case, however, we look for the orthogonal projection of  $b$  onto the linear subspace  $\text{im } A$  within  $\mathbb{R}^m$ , see fig. 3.1.

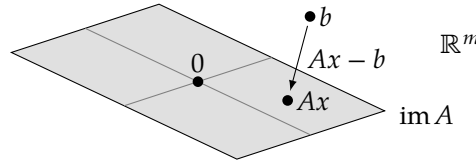


Figure 3.1: When we orthogonally project  $b$  onto the linear subspace  $\text{im } A$  of  $\mathbb{R}^m$ , we hit a certain  $Ax$  which minimizes  $\|Ax' - b\|$  among all  $x' \in \mathbb{R}^n$ .

Assume that  $x$  fulfills the property that  $Ax$  is the orthogonal projection of  $b$  onto  $\text{im } A$ . Then any vector in  $\text{im } A$  is orthogonal to  $(Ax - b)$ , which means that their inner product is zero. Hence, for any  $x' \in \mathbb{R}^n$  it holds that

$$(Ax') \cdot (Ax - b) = 0.$$

Let us denote by  $A^\dagger$  the transpose of the matrix  $A$ . We recall that  $(AB)^\dagger = B^\dagger A^\dagger$  for matrices  $A$  and  $B$ , and therefore  $A \cdot x' = x' \cdot A^\dagger$ , where  $x'$  first denotes a column vector and then a row vector. We conclude that for any  $x' \in \mathbb{R}^n$

$$x' \cdot A^\dagger (Ax - b) = 0$$

This is indeed the case if  $A^\dagger (Ax - b)$  is zero, which means  $A^\dagger Ax = A^\dagger b$ . In other words, we look for a solution  $x$  of the so-called *normal equation system*

$$(A^\dagger A) \cdot x = (A^\dagger b). \quad (3.7)$$

Hence, any  $x \in \mathbb{R}^n$  that solves eq. (3.7) minimizes  $\|Ax - b\|$ . In general the solution  $x$  is not unique. However, if  $A$  has maximal rank – so the columns are linearly independent – then it

<sup>5</sup>In Jan 01, 1801 the asteroid Ceres was discovered and tracked for 40 days, until it vanished behind the sun. It was the 24-year old Gauss who could predict its future position using least squares, which allowed to relocate Ceres again.

<sup>6</sup>In fact, for a linear model of data points with Gaussian distributed errors the least square method yields the maximum likelihood estimator.

<sup>7</sup>Dt. Untervektorraum

can be shown that  $A^\dagger A$  is regular and the solution  $x$  is unique. (This follows from  $\text{rank } A = \text{rank } A^\dagger A$ , see [18] for details.)

Note that if  $A$  has maximal rank such that  $A^\dagger A$  is regular then we can directly calculate

$$x = (A^\dagger A)^{-1} A^\dagger \cdot b \quad (3.8)$$

as the “best solution” of the overdetermined system  $Ax = b$  in the sense that the error  $\|Ax - b\|$  is minimized. Hence,  $(A^\dagger A)^{-1} A^\dagger$  plays the role of an “inverse” of  $A$  although  $A$  is not necessarily regular, not even square. In fact, if  $A$  has maximal rank then  $(A^\dagger A)^{-1} A^\dagger$  goes by the name *pseudoinverse* or *Moore-Penrose inverse*<sup>8</sup> of  $A$ . The pseudoinverse is closely linked to the *singular value decomposition*, see [21] for details.

One of numerous applications of the pseudoinverse is the computation of the inverse of a Jacobian matrix that arises in the multi-dimensional Newton-Raphson method when searching for roots of functions. This is, for instance, the basis of a numerical method for the backward kinematics in robotics. Another example is presented in the following section.

### 3.3.3 Fitting functions

#### Linear regression

The term “regression” in *linear regression* has a historical background: Francis Galton studied the heights of adults as a function of their parent’s height and found a tendency, namely *regression to the mean*. Galton essentially got a plot of points  $(x_1, y_1), \dots, (x_m, y_m) \in \mathbb{R}^2$  as in fig. 3.2 and asked for the best fitting linear function.

By “best fitting” we mean that we assume a linear model  $f(x) = k \cdot x + d$  for the data and we want to find the parameters  $k, d \in \mathbb{R}$  such that the (sum of squares) error  $\sum_i (f(x_i) - y_i)^2$  is minimized. Phrasing the problem like this makes it compatible with the framework of overdetermined linear equation systems, namely  $f(x_i) = y_i$  for all  $1 \leq i \leq m$ , or in matrix notation:

$$\underbrace{\begin{pmatrix} 1 & x_1 \\ \vdots & \vdots \\ 1 & x_m \end{pmatrix}}_A \cdot \begin{pmatrix} d \\ k \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix} \quad (3.9)$$

If not all  $x_i$  are equal then  $A$  has rank 2, which is maximal, and by virtue of eq. (3.8) we can directly calculate the parameter vector

$$\begin{pmatrix} d \\ k \end{pmatrix} = (A^\dagger A)^{-1} A^\dagger \cdot \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}$$

from eq. (3.8) for the function  $f(x) = kx + d$  plotted in fig. 3.2. If  $m = 2$  and  $x_1 \neq x_2$  then  $A$  is regular. As a consequence  $(A^\dagger A)^{-1} A^\dagger = A^{-1}$  and we obtain the one linear function that passes through the two points. If all  $x_i$  are equal then  $A^\dagger A$  is singular<sup>9</sup>. Then eq. (3.7) has infinitely many solutions and there are infinitely many best fitting functions.<sup>10</sup>

<sup>8</sup>Note that we only considered overdetermined systems here. However, the Moore-Penrose inverse can also be defined for underdetermined systems, in fact it uniquely exists for any matrix  $A$ .

<sup>9</sup>Not regular, not invertible.

<sup>10</sup>If all  $x_i$  are equal then every best fitting linear function passes through a point  $(x_i, y)$ , and every linear function that passes through that point is best fitting as it has the same error. This point  $(x_i, y)$  therefore minimizes  $\sum_i (y_i - y)^2$ , which gives  $y = 1/m \sum_i y_i$ . So the point  $(x_i, y)$  is the center of gravity of the data points.

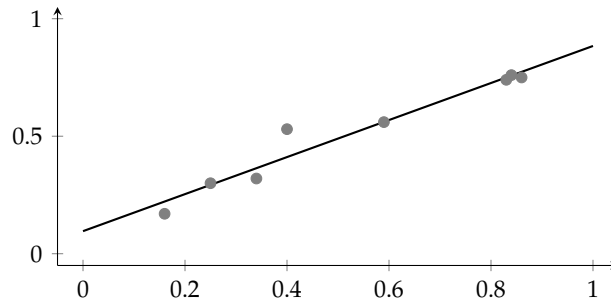


Figure 3.2: Eight data points give rise to an overdetermined linear equation system for a fitting linear function.

### General regression

We can generalize this idea of fitting functions as follows. If we recap eq. (3.9) then we can interpret this equation as follows: We have a linear combination of two base functions, the constant function  $g_1(x) = 1$  and the function  $g_2(x) = x$ , and we want to find the coefficients  $k$  and  $d$  of this linear combination that minimizes the least square error.

The general idea is to consider  $n$  base functions  $g_1, \dots, g_n$  and ask for the linear combination  $f = \sum_{i=1}^n \alpha_i g_i$  for the data points  $(x_1, y_1), \dots, (x_m, y_m)$  such that the error

$$\sum_{i=1}^m (f(x_i) - y_i)^2 = \sum_{i=1}^m \left( \sum_{j=1}^n \alpha_j g_j(x_i) - y_i \right)^2$$

is minimized. This again is the solution of the overdetermined linear equation system

$$\underbrace{\begin{pmatrix} g_1(x_1) & \cdots & g_n(x_1) \\ \vdots & & \vdots \\ g_1(x_m) & \cdots & g_n(x_m) \end{pmatrix}}_A \cdot \begin{pmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}. \quad (3.10)$$

The set of linear combinations of the  $g_i$  span a vector space of functions and it makes sense that the  $g_i$  form a *basis*<sup>11</sup> of this vector space, i.e., they shall be linearly independent. Otherwise the columns of  $A$  in eq. (3.10) will not be linearly independent and  $A$  cannot have maximal rank.

Note that the  $g_i$  do not need to be linear functions. We could choose the base functions  $1, \sin(x), \cos(x), \dots, \sin(nx), \cos(nx)$  and span the vector space of all trigonometric polynomials up to degree  $n$ . This way we create a conceptional bridge between the Fourier transform and fitting of functions.

A very practical choice of base functions is  $1, x, x^2, \dots, x^n$  to form polynomials of the form  $\sum_{i=0}^n \alpha_i x^i$ . We call this *polynomial regression*. These base functions span the vector space of polynomial functions up to degree  $n$ . In this case eq. (3.10) yields

$$\begin{pmatrix} 1 & x_1 & x_1^2 & \cdots & x_1^n \\ \vdots & \vdots & \vdots & & \vdots \\ 1 & x_m & x_m^2 & \cdots & x_m^n \end{pmatrix} \cdot \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_n \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_m \end{pmatrix}. \quad (3.11)$$

<sup>11</sup>The vectors  $v_1, \dots, v_d$  of a vector space  $V$  (of finite dimension) form a *basis* if they span  $V$  – the set of linear combinations fills  $V$  out – and they are linearly independent. So a basis is a smallest set of linearly independent vectors that span  $V$ . Every basis of  $V$  has the same number of elements, which is called the *dimension* of  $v$ . Also functions can form vector spaces, e.g., the set of functions  $\mathbb{R} \rightarrow \mathbb{R}$  forms a vector space  $V$ , where  $(f + g)(x) = f(x) + g(x)$  and  $(\lambda f)(x) = \lambda \cdot f(x)$  for all  $f, g \in V$  and  $\lambda \in \mathbb{R}$ .

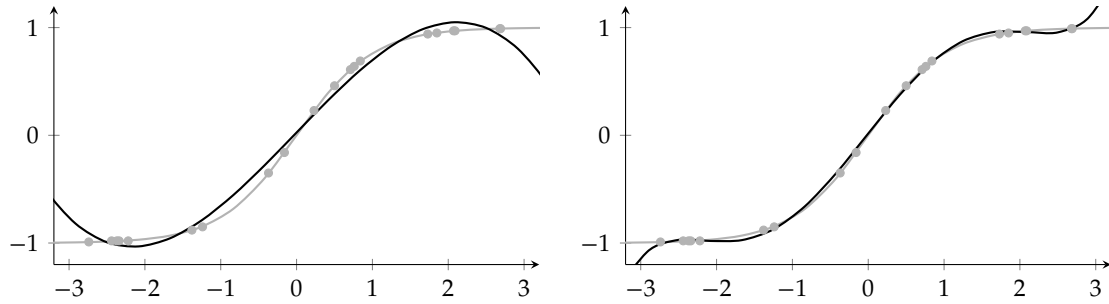


Figure 3.3: Polynomial fit of data points that sample  $\tanh$  at 20 uniformly random points on  $[-3, 3]$ . Left: The polynomial of degree 3. Right: The polynomial of degree 5.

and the solution leads to the best approximating polynomial function up to degree  $n$ . The initial example of fitting a linear function is a polynomial fit with  $n = 1$ , see eq. (3.9) versus eq. (3.11). In fig. 3.3 two examples of approximating polynomials are given. They have both been computed by eq. (3.8) applied to eq. (3.11).

Software packages like numpy for Python or MATLAB provide library functions that implement least square polynomial fit. The following lines are from a Python interpreter shell:

```
>>> import numpy as np
>>> x = np.array([0.0, 1.0, 2.0, 3.0, 4.0, 5.0])
>>> y = np.array([0.0, 0.8, 0.9, 0.1, -0.8, -1.0])
>>> z = np.polyfit(x, y, 3)
>>> z
array([ 0.08703704, -0.81349206,  1.69312169, -0.03968254])
>>> print(np.poly1d(z))
          3          2
0.08704 x - 0.8135 x + 1.693 x - 0.03968
```

### Supervised learning

In an even more generalized setting we end up in *supervised machine learning*. We are given a *training set* of inputs  $x_i \in \mathbb{R}^n$  and desired outputs  $y_i \in \mathbb{R}^m$ , which are sometimes called *labels*.

We want to model the relationship between the input and the output by certain functions  $f: \mathbb{R}^n \rightarrow \mathbb{R}^m$ , such as feed-forward neural nets. We describe this function  $f$  through a list of parameters  $\theta$ , like the weights in the neural net. That is, we consider a whole family of models  $f_\theta$  and look for the parameters  $\theta$  that yield the model that describes the data best. In machine learning, the error is called *loss* and often denoted by  $\ell$ . A common choice is the 2-norm

$$\ell = \sum_i (y_i - f_\theta(x_i))^2.$$

We now look for the parameters  $\theta$  that minimize the loss  $\ell$ . However, interesting families of models are too complex such that we can directly compute the optimum via the Moore-Penrose inverse. Instead, numerical optimization is applied, such as *stochastic gradient descent* (SGD) or adaptive versions of it, like Adam or AMSGrad. This is called *training* in machine learning.



### 3.3.4 QR decomposition

The QR decomposition is a method that can solve regular linear equation systems and overdetermined linear equation systems. It can be shown that the condition of the QR decomposition is significantly better than the one of the normal equations. It also introduces less rounding errors than Gaussian elimination.

We again consider a linear equation system  $Ax = b$  with a  $m \times n$  matrix  $A$ , where  $m \geq n$ . It can be shown that there is always an  $m \times m$  orthogonal matrix  $Q$  such that

$$QA = \begin{pmatrix} R \\ 0 \end{pmatrix}, \quad (3.12)$$

where  $R$  is a  $n \times n$  right triangular matrix and  $0$  is a  $(m - n) \times n$  zero matrix.

Recall that a square matrix is called orthogonal if its columns are orthogonal unit vectors, i.e., they form an orthonormal basis of the  $\mathbb{R}^m$ . From that it follows that  $Q^\dagger Q = QQ^\dagger = I$  which means that  $Q$  can be trivially inverted as  $Q^\dagger = Q^{-1}$ . An orthogonal matrix  $Q$  also has the nice property that it does not change the length of vectors, i.e.,  $\|Qx\| = \|x\|$ . In some sense,  $Q$  is only performing combinations of rotations and reflections.

The question is now how to solve  $A \cdot x = b$  given the above QR decomposition, i.e., what  $x$  is minimizing  $\|A \cdot x - b\|$ ? Note that  $Q$  does not change lengths of vectors, so we can actually minimize  $\|QA \cdot x - Qb\|$  instead. Assume we know  $Q$  then we can also compute

$$Qb = \begin{pmatrix} c \\ d \end{pmatrix}$$

with a vector  $c \in \mathbb{R}^n$  and  $d \in \mathbb{R}^{m-n}$ . Now we observe that for any  $x \in \mathbb{R}^n$

$$\|Ax - b\|^2 = \|Q(Ax - b)\|^2 = \|QAx - Qb\|^2 = \left\| \begin{pmatrix} Rx - c \\ -d \end{pmatrix} \right\|^2 = \|Rx - c\|^2 + \|d\|^2 \geq \|d\|^2. \quad (3.13)$$

Hence, the left-hand side is minimized exactly when  $Rx = c$ . We therefore look for the solution  $x$  of  $Rx = c$  to minimize  $\|Ax - b\|$ . Now remember that  $R$  is a right triangular matrix and hence  $Rx = c$  is easy to solve via back substitution. This method is called *QR method* because  $A$  can be expressed as

$$A = Q^\dagger \begin{pmatrix} R \\ 0 \end{pmatrix}. \quad (3.14)$$

The essential step in the QR method is the computation of the matrix  $Q$ . A numerically stable algorithm to compute  $Q$  is based on so-called Householder reflections. Reflection matrices  $Q_1, \dots, Q_n$  are applied to  $A$  in a way such that the  $Q_k$  basically generates the  $k$ -th column of the right-hand side in eq. (3.12). The product  $Q_n \cdots Q_1$  is then  $Q$  in eq. (3.12). The other algorithm uses so-called Givens rotations rather than Householder reflections.

Software packages like numpy for Python or MATLAB provide library functions that implement QR decomposition. The following lines are from a Python interpreter shell. (Note that `np.linalg.qr()` returns the two factors in the right-hand side of eq. (3.14).)

```
>>> import numpy as np
>>> A = np.random.randn(9, 6)           # Random 9x6 matrix
>>> Q, R = np.linalg.qr(A)
>>> np.linalg.norm(A - Q @ R) <= 1e-14  # A == QR
True
```

Besides the QR decomposition there are a couple of other common matrix decompositions. For instance, any square matrix  $A$  admits an *LU decomposition*

$$A = P \cdot L \cdot U,$$

where  $P$  is a permutation matrix,  $L$  is a left (lower) triangular matrix and  $U$  is an upper (right) triangular matrix. This decomposition is typically used to solve regular linear equation systems, like the function `np.linalg.solve()` does in numpy. In MATLAB the function `linsolve()` uses LU decomposition if the coefficient matrix  $A$  is square and QR decomposition in all other cases.

### 3.3.5 Equilibration and regularization

In the row reduction steps of the Gaussian elimination method we multiplied single equations without changing the set of solutions. The solution of an overdetermined system of equations, however, is only an approximate solution that minimizes the least square error. Hence, if we scale a single equation then we change the expression for the error and we obtain a different solution.

More precisely, let  $A \cdot x = b$  denote an overdetermined system and let  $x$  be a solution. We learned from section 3.3.1 that  $x$  therefore minimizes the error expression

$$\|Ax - b\|^2 = \sum_{i=1}^m \left( \sum_{j=1}^n a_{ij}x_j - b_i \right)^2,$$

where  $A = (a_{ij})$  and  $b = (b_i)$ . Assume now that we multiply the  $k$ -th equation by a factor  $\lambda \neq 0$ . We therefore obtain a new matrix  $A' = (a'_{ij})$  and a new right-hand side  $b'_i$  with

$$a'_{ij} = \begin{cases} a_{ij} & \text{for } i \neq k \\ \lambda a_{ij} & \text{for } i = k \end{cases} \quad \text{and} \quad b'_i = \begin{cases} b_i & \text{for } i \neq k \\ \lambda b_i & \text{for } i = k \end{cases}.$$

The solution  $x'$  to this new system now minimizes the error expression

$$\sum_{i \neq k} \left( \sum_j a_{ij}x_j - b_i \right)^2 + \lambda^2 \left( \sum_j a_{kj}x_j - b_k \right)^2.$$

In other words, the solution  $x'$  now puts a *weight*  $\lambda$  on the  $k$ -th equation for the error minimization. By adjusting  $\lambda$  we can control how important or significant an equation is to us.

**Equilibration.** Assume that we actually have  $m = m_1 + m_2$  equations in our system, where the first  $m_1$  equations stem from a certain objective to be optimized and a second set of  $m_2$  equations that stem from a different objective. Assume that both objectives are equally important to us, but  $m_1 \neq m_2$ . We scale the first  $m_1$  equations by  $1/m_1$  and the others by  $1/m_2$  such that the sum of weights for the equations of each objective is 1, which results in the error expression

$$\frac{1}{m_1} \sum_{i=1}^{m_1} \left( \sum_j a_{ij}x_j - b_i \right)^2 + \frac{1}{m_2} \sum_{i=m_1+1}^{m_1+m_2} \left( \sum_j a_{ij}x_j - b_i \right)^2.$$

*Equilibration* is the method of scaling equations in a way to equilibrate their weight. Depending on the problem we may, for instance, scale the equations such that the coefficient vectors  $(a_{k1}, \dots, a_{kn})$  are all of equal length for  $1 \leq k \leq m$ . This way all equations obtain a kind of “unit weight”.

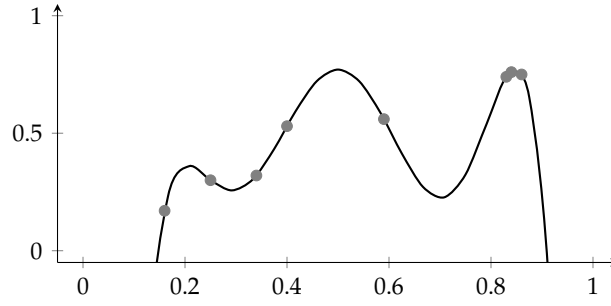


Figure 3.4: The polynomial of degree 6 fitting 8 data points shows strong oscillations.

**Regularization.** For certain systems the solution may not “behave very well”. Consider for instance the polynomial of degree 6 that is shown in fig. 3.4 and fits the point set from fig. 3.2. What we see is the typical behavior of polynomials of higher degree: They have a strong tendency to oscillate significantly.

In order to counteract against this effect we can “penalize” the oscillation behavior by extending the error term accordingly. By “oscillation” we actually mean high curvature and in fact the *strain energy* of a function  $f: \mathbb{R} \rightarrow \mathbb{R}$  in the interval  $[a, b]$  is given by

$$\int_a^b f''(x)^2 \, dx, \quad (3.15)$$

which we could interpret as the infinitesimal sum (integral) of the square error of the curvature (second derivative). We have a polynomial  $f(x) = \sum_{i=1}^n \alpha_i x^i$  whose second derivative is

$$f''(x) = \sum_{i=2}^n \alpha_i x^{i-2} \cdot i(i-1) \quad (3.16)$$

We would like to minimize the error term given in eq. (3.15) for the  $\alpha_k$ , so we set the partial derivatives to zero. We see from eq. (3.16) that  $\alpha_0, \alpha_1$  actually do not matter so we only consider the  $n-1$  equations for  $\alpha_2, \dots, \alpha_n$ :

$$\begin{aligned} 0 &= \frac{\partial}{\partial \alpha_k} \int_a^b \left( \sum_{i=2}^n \alpha_i x^{i-2} \cdot i(i-1) \right)^2 \, dx \\ &= \int_a^b 2 \cdot \left( \sum_{i=2}^n \alpha_i x^{i-2} \cdot i(i-1) \right) x^{k-2} \cdot k(k-1) \, dx \\ &= 2 \cdot \sum_{i=2}^n \alpha_i \cdot ik(i-1)(k-1) \cdot \int_a^b x^{i+k-4} \, dx \\ &= 2 \cdot \sum_{i=2}^n \alpha_i \cdot ik(i-1)(k-1) \frac{b^{i+k-3} - a^{i+k-3}}{i+k-3} \end{aligned}$$

We end up with a system of  $n-1$  linear equations

$$(c_{ki}) \cdot (\alpha_i) = 0 \quad \text{where} \quad c_{ki} = \begin{cases} 0 & \text{for } i \leq 2 \\ ik(i-1)(k-1) \frac{b^{i+k-3} - a^{i+k-3}}{i+k-3} & \text{for } i > 2 \end{cases} \quad (3.17)$$

and  $k$  ranging from 2 to  $n$ . Here  $(c_{ki})$  and  $(\alpha_i)$  denote matrices and vectors, respectively.

However, we want to control the amount of this penalty and therefore we weight them by a weight  $\lambda > 0$ . Together with the original system of eq. (3.11) for the approximation of the data points, we end up with the following system:

$$\begin{pmatrix} 1 & x_1 & x_1^2 & \dots & x_1^n \\ 1 & x_m & x_m^2 & \dots & x_m^n \\ 0 & 0 & \lambda c_{22} & \dots & \lambda c_{2n} \\ 0 & 0 & \lambda c_{n2} & \dots & \lambda c_{nn} \end{pmatrix} \cdot \begin{pmatrix} \alpha_0 \\ \vdots \\ \alpha_n \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_m \\ 0 \\ \vdots \\ 0 \end{pmatrix}. \quad (3.18)$$

The first  $m$  equations stem from the approximation task of the data points and the next  $n - 1$  equations stem from the curvature penalty. The error term minimized by the entire system is

$$\sum_{k=1}^m (f(x) - y_i)^2 + \lambda^2 \int_a^b f''(x)^2 dx.$$

If we choose  $\lambda > 0$  then the solution becomes more *regular* in the sense of “well-behaved”. Therefore we call  $\lambda^2 \int_a^b f''(x)^2 dx$  the *regularization term* and the method is called *regularization*. If we choose  $\lambda = 0$  then we have the original non-regularized version, see fig. 3.5 for an example. Of course, increasing  $\lambda$  reduces the amount of oscillation at the expense of an increased approximation error. Furthermore, we would like to combine this regularization with equilibration, such that the effect of parameter  $\lambda$  becomes somewhat independent of  $m$ .

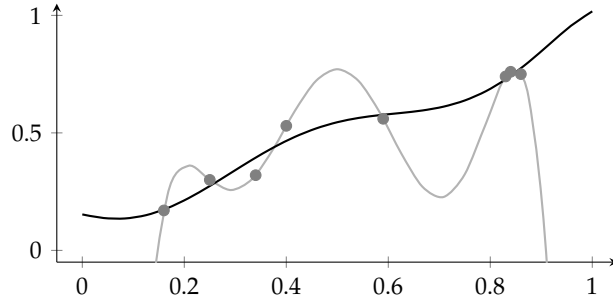


Figure 3.5: Regularized solution for a polynomial of degree 6 as in fig. 3.4. The black graph shows the result for  $\lambda = 0.001$  and the gray graph for  $\lambda = 0$ , which equals therefore the non-regularized version. The strain energy is computed over the interval  $[0, 1]$ .

**Regularizing training of neural nets.** Similar ideas to equilibration and regularization is applied when training neural nets. In particular deep neural nets possess many model parameters, which are to be trained through gradient descent optimization, see section 3.3.3.

This gives those nets a high learning capacity but they are also prone to overfitting leading to exactly the behavior as illustrated in fig. 3.4. This oscillating behavior hurts the generalization capability of the neural net, because similar input leads to strongly different output.

To mitigate overfitting (and to stabilize gradient descent training), a standard technique is to add  $L_1$ - or  $L_2$ -regularization: It causes a normalization of the weight vectors formed by the weights of neurons. This is similar to normalizing the coefficient vectors as described above for equilibration and causes a smoothed behavior as illustrated for regularization in fig. 3.5.

# Polynomial interpolation

## 4.1 Motivation

We often face the situation, where a function  $f$  is not given by a closed expression, but at finitely many positions  $x_1, \dots, x_n$  and we want to evaluate  $f$  at arbitrary positions  $x$ . In engineering the pairs  $(x_i, f(x_i))$  often stem from measurements. A typical approach to this task is to approximate  $f$  by a polynomial  $p$  with  $p(x_i) = f(x_i)$  for all  $1 \leq i \leq n$  and evaluate  $p(x)$  as an approximation for  $f(x)$ . The  $x_i$  are called (*interpolation*) *nodes*<sup>1</sup>. Typically  $x$  is in the interval between the smallest and the largest node. If  $x$  is outside this interval then we also speak of an *extrapolation*.

But interpolation is not only useful when the input stems from measurements: Consider a parallel curve (of small distance) to the function graph of  $x^2$ . This curve is again the function graph of a function  $f$ , for which it might be difficult to find a simple expression, but we can approximate it using a finite number of samples. Strictly speaking, if we can choose the interpolation points then we actually speak of *function approximation* rather than interpolation.

Let us further assume that we now would like to integrate or differentiate a function  $f$ . Even if  $f$  is given by a closed expression, integration or differentiation might be difficult. After all, there is for instance no elementary function for the integral of  $e^{-x^2}$ . The integration and differentiation of polynomials is easy, so we could again approximate  $f$  by a polynomial and integrate or differentiate the polynomial instead. Interpolation is therefore also the basis for further numerical methods and the question arises what error is introduced by the polynomial approximation. In general, numerical computation is much easier than symbolic computation.

Instead of polynomials we could also use other simple and versatile functions for interpolation, like linear combinations of trigonometric functions. Here we restrict ourselves to polynomials. After all, the Stone-Weierstrass approximation theorem says that every continuous function defined on a closed interval  $[a, b]$  actually can be (uniformly) approximated by polynomials, which is all but clear.<sup>2</sup>

## 4.2 Power series

Polynomials play an important role for approximation because they are able to represent an important class of functions. A function  $f: \mathbb{R} \rightarrow \mathbb{R}$  is called *analytic* on the open set  $D \subseteq \mathbb{R}$  if it can

<sup>1</sup>Dt. Stützstelle

<sup>2</sup>More precisely, let  $f: [a, b] \rightarrow \mathbb{R}$  be continuous and let  $\varepsilon > 0$  be arbitrarily small. Then there is a polynomial function  $p$  such that  $\|f - p\| < \varepsilon$ , where  $\|\cdot\|$  denotes the supremum norm. Put in words of topology: The set of polynomial functions is dense in the set of continuous functions over  $[a, b]$ .

be represented by a *power series*<sup>3</sup>

$$f(x) = \sum_{k=0}^{\infty} a_k (x - x_0)^k, \quad (4.1)$$

such that  $x_0$  can be chosen arbitrarily from  $D$ . All elementary functions are analytic on  $\mathbb{R}$ : Polynomials, exponential function, logarithms, and the trigonometric functions. Sums, products and compositions of analytic functions are again analytic.

The *Taylor series* tells us how to obtain the coefficients  $a_n$  in eq. (4.1):

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(x_0)}{k!} (x - x_0)^k.$$

Hence, analytic functions have this incredible property that if we know all derivatives at a single location  $x_0$  then we globally know the function at any  $x$  in the domain.

Not all processors provide machine instructions for the exponential, logarithmic or trigonometric functions. But even if they do, they might be inaccurate or we would like to trade accuracy versus speed. Or maybe we would like to implement these functions in an FPGA using addition and multiplication only. In such cases, Taylor series are a common method to approximate these functions by just using the first  $n$  summands. For instance

$$\exp(x) \approx \sum_{k=0}^n \frac{x^k}{k!} \quad \text{and} \quad \sin(x) \approx \sum_{k=0}^n (-1)^k \frac{x^{2k+1}}{(2k+1)!}.$$

Even  $\sin(x) \approx x$  is accurate up to a relative error of 1 % in the interval  $[-0.25, 0.25]$ .

## 4.3 Single interpolation polynomials

### 4.3.1 Existence

A polynomial of degree  $n - 1$  can exactly interpolate  $n$  points. More precisely, let  $x_1, \dots, x_n$  be pairwise distinct real numbers and let  $y_1, \dots, y_n$  be real numbers. Then there is exactly one polynomial  $p$  of degree at most  $n - 1$  such that

$$p(x_i) = y_i \quad (4.2)$$

for all  $1 \leq i \leq n$ . In particular, a constant function (polynomial of degree 0) can interpolate one point, a linear function (polynomial of degree 1) can interpolate two points, and so on. We can compute  $p$  by considering the linear equation system behind eq. (4.2), namely

$$\begin{pmatrix} 1 & x_1 & \dots & x_1^{n-1} \\ & & \ddots & \\ 1 & x_n & \dots & x_n^{n-1} \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ \vdots \\ a_{n-1} \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}, \quad (4.3)$$

where  $p(x) = \sum_{k=0}^{n-1} a_k x^k$ . The coefficient matrix is regular if its determinate is nonzero. This determinate is known as the *Vandermonde determinant*. It has the value

$$\prod_{1 \leq i < k \leq n} (x_k - x_i)$$

and is non-zero for pairwise distinct  $x_i$ . We call the  $x_i$  the *nodes* and the unique  $p$  the *interpolation polynomial*.

---

<sup>3</sup>Dt. Potenzreihe

### 4.3.2 Interpolation error

Let us consider a function  $f: I \rightarrow \mathbb{R}$  on an interval  $I = [a, b]$  and pairwise distinct interpolation nodes  $x_1, \dots, x_n$ . We know that there is a unique interpolation polynomial  $p$  of degree at most  $n - 1$  such that  $p(x_i) = f(x_i)$  for all  $1 \leq i \leq n$ . But what can we say about the error, i.e., the difference  $f(x) - p(x)$  for  $x \in I$ ?

First, we define by  $\|f\|$  the *maximum norm* of  $f$  as

$$\|f\| = \max_{x \in I} |f(x)|.$$

Next we define the *node polynomial*  $w$  by

$$w(x) = \prod_{i=1}^n (x - x_i).$$

It can be shown that for any  $x$  there is some  $\xi \in I$  such that

$$f(x) - p(x) = \frac{f^{(n)}(\xi)}{n!} \cdot w(x) \quad (4.4)$$

for all  $x \in I$ . Even if we do not know how to compute  $\xi$ , we can conclude that

$$\|f - p\| \leq \frac{1}{n!} \|f^{(n)}\| \|w\|. \quad (4.5)$$

The left-hand side of eq. (4.5) is the maximum interpolation error on  $I$ , which is  $\max_{x \in I} |f(x) - p(x)|$ . This term is bound by the right-hand side, which is small if  $\|w\|$  is small. If we can choose the interpolation nodes  $x_i$  then we can choose them in a clever way such that  $\|w\|$  becomes small. If we choose the interpolation nodes uniformly on our interval  $I$  then  $w(x)$  tends to become large at the boundary of  $I$ , see fig. 4.1. More precisely, the extreme values of  $w$  get larger towards the boundary of  $I$ . This is known as *Runge's phenomenon*.

If we, however, redistribute the nodes to increase the density of the nodes towards the boundary of  $I$  then the extreme values of  $w$  get balanced. In fact, it can be shown that setting

$$x_i = \cos \frac{2i-1}{2n} \pi \quad (4.6)$$

makes the extreme values of  $w$  all equal, namely  $1/2^{n-1}$ , which in this sense is optimal for a polynomial interpolation on  $I = [-1, 1]$ , see fig. 4.1. The nodes given by eq. (4.6) are called *Chebyshev nodes* and they are the roots of the so-called *Chebyshev polynomial* of  $n$ -th degree. If we insert this into eq. (4.5), for Chebyshev nodes we therefore get an error bound of

$$\|f - p\| \leq \frac{\|f^{(n)}\|}{n! 2^{n-1}}. \quad (4.7)$$

In general, increasing the number  $n$  of nodes has only limited effect in improving the interpolation error. The reason is that polynomials of higher degree have a strong tendency for oscillation, as we already observed in fig. 3.4 in chapter 3. In fig. 4.2 an interpolation polynomial is shown that also illustrates this behavior.

In fact, it can happen that the interpolation error does not converge to zero when we increase  $n$  towards infinity. The reason is that in eq. (4.5) the term  $\|f^{(n)}\|$  can grow towards  $\infty$  faster than  $\|w\|/n!$  goes to zero.

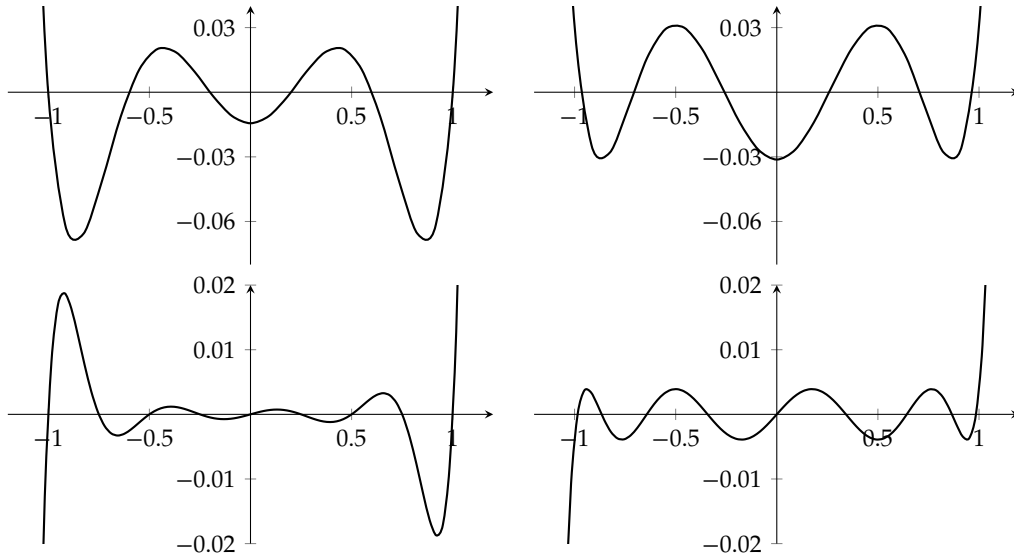


Figure 4.1: The node polynomial  $w(x)$ . Top: Polynomials of degree 6. Bottom: Polynomials of degree 9. Left: Uniform nodes on  $[-1, 1]$ . Right: Chebyshev nodes.

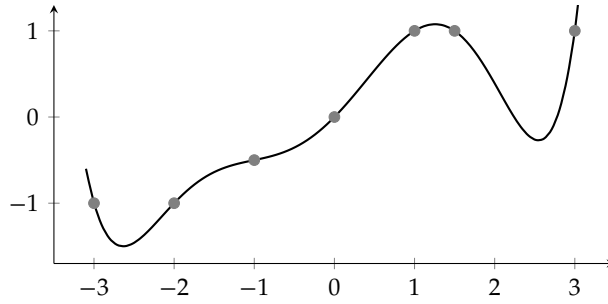


Figure 4.2: An interpolation polynomial of degree 6 that shows typical oscillation behavior.

### 4.3.3 Computing interpolation polynomials

In this section, we will introduce two different methods to compute interpolation polynomials: Lagrange's formulas and the Neville tableau. Of course, it would be possible to compute the interpolation polynomial by solving the linear system in eq. (4.3), but we can in fact compute them directly without paying the costs of solving a linear system of equations.

#### Lagrange's formula

We want to find a polynomial  $p$  of degree  $n - 1$  with  $p(x_k) = y_k$  for all  $1 \leq k \leq n$ . The idea is now that we construct for each such  $k$  a polynomial  $L_k$  of degree  $n - 1$  that is 1 at  $x_k$ , but 0 at all other nodes, i.e.,  $L_k(x_i) = \delta_{ik}$ . This directly leads to the sought interpolation polynomial

$$p(x) = \sum_{k=1}^n y_k L_k(x), \quad (4.8)$$



because

$$p(x_i) = \sum_{k=1}^n y_k \delta_{ik} = y_i \delta_{ii} = y_i.$$

The polynomials  $L_k$  are called *Lagrange polynomials* of degree  $n$  and the property  $L_k(x_i) = \delta_{ik}$  is easily checked for their definition:

$$L_k(x) = \prod_{\substack{i=1 \\ i \neq k}}^n \frac{x - x_i}{x_k - x_i}. \quad (4.9)$$

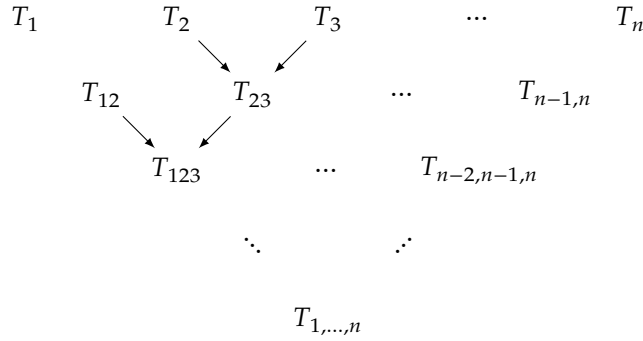
Plugging everything together gives *Lagrange's formula* for the interpolation polynomial:

$$p(x) = \sum_{k=1}^n \prod_{\substack{i=1 \\ i \neq k}}^n \frac{x - x_i}{x_k - x_i} y_k.$$

### Neville tableau

The Lagrange formula is easy to understand, but the following *Neville algorithm* is better suited for implementation. In particular, it allows to give an error estimate of the result, see [21] for details. It follows the classical approaches of *divide and conquer* and *dynamic programming* for algorithm design: We solve the same problem for smaller instances first and then plug the sub-results together to form the solution of larger instances.

More precisely, we start with interpolation polynomials  $T_i(x) = y_i$  of degree 0 that only interpolate a single node  $y_i$ . We then combine them in a way to form polynomials  $T_{i,i+1}$  of degree 1 that interpolate two nodes  $x_i, x_{i+1}$ , and so on. In general,  $T_{i,\dots,k}$  interpolates  $x_i, \dots, x_k$  and eventually we obtain  $T_{1,\dots,n}$  that interpolates all nodes  $x_1, \dots, x_n$ . We end up with a tableau of this form:



Each element is recursively defined by its two ancestors above, except for the first row:

$$T_i(x) = y_i \quad (4.10)$$

$$T_{i,\dots,i+m}(x) = \frac{(x - x_{i+m})T_{i,\dots,i+m-1}(x) + (x_i - x)T_{i+1,\dots,i+m}(x)}{x_i - x_{i+m}}. \quad (4.11)$$

Plainly implementing this recursion leads to many re-computations of the same sub-results, i.e.,  $T_2$  is reached in multiple ways in the above tableau. A standard technique of dynamic

programming is *memoization*: We remember the sub-results instead of re-computing them. This makes the total effort proportional to the size of the tableau.

Note that in the above recursion each  $T_{i,\dots,i+m}$  results from a *linear interpolation* of the two ancestors  $T_{i,\dots,i+m-1}$  and  $T_{i+1,\dots,i+m}$ . In particular, the elements  $T_{i,i+1}$  in the second row form a linear interpolation between  $y_i$  and  $y_{i+1}$ :

$$T_{i,i+1} = \frac{(x - x_{i+1})y_i + (x_i - x)y_{i+1}}{x_i - x_{i+1}} \quad (4.12)$$

The first row in the tableau,  $T_1, \dots, T_n$ , does not need to be in any particular order. We could also easily add a new interpolation node and update the tableau without recomputing it entirely. We just add a new (diagonal) column in the tableau. Sometimes it therefore makes sense to sort the  $T_1, \dots, T_n$  in increasing distance to the position  $x$  and keep adding interpolation points until the changes drop below a certain threshold, instead of computing the entire final tableau.

## 4.4 Splines

### 4.4.1 Motivation

We learned in section 4.3 that polynomials of high degree tend to oscillate, as illustrated in fig. 4.2. For certain applications we could, of course, use a piecewise linear function that interpolates between the points. So let  $x_1 < \dots < x_n$  denote  $n$  nodes with function values  $y_1, \dots, y_n$ . As illustrated in fig. 4.3a, for each  $1 \leq i \leq n-1$  we put a linear functions  $p_i$  on the interval  $[x_i, x_{i+1}]$  that linearly interpolates between the nodes  $x_i$  and  $x_{i+1}$ :

$$p_i(x) = \lambda y_i + \mu y_{i+1} \quad \text{with} \quad \lambda = \frac{x - x_{i+1}}{x_i - x_{i+1}} \quad \text{and} \quad \mu = 1 - \lambda = \frac{x_i - x}{x_i - x_{i+1}}.$$

These are exactly the polynomials  $T_{i,i+1}$  of the first row in the Neville tableau, see also eq. (4.12).

Many applications, however, require an interpolation function that is at least twice differentiable, in particular for applications in physics and engineering. For instance, a co-called cam profile tells how a secondary servo drive (slave axis) should move in dependence of a first servo drive (master axis). A cam profile therefore maps one position to another and they are often given in tabulated form  $(x_1, y_1), \dots, (x_n, y_n)$  such that we have to compute an interpolation. The second derivative  $f''$  of the interpolating function  $f$  relates<sup>4</sup> to the acceleration, which must be finite.

The idea is to generalize piecewise linear functions to piecewise polynomial functions that fulfill certain additional properties, like being twice differentiable. Such functions are called *splines*. In this sense, a piecewise linear function is a spline of degree 1. A step function (piecewise constant) would be a spline of degree 0. By far the most common variant, however, is the cubic spline, which is of degree 3.

### 4.4.2 Cubic splines

By a cubic spline  $f$  we mean a twice continuously differentiable spline of degree three that interpolates a tabulated function  $(x_1, y_1), \dots, (x_n, y_n)$ . That is, the second derivative of a cubic spline

<sup>4</sup>If the master axis moves at unit speed then the second derivative is exactly the acceleration of the slave axis.

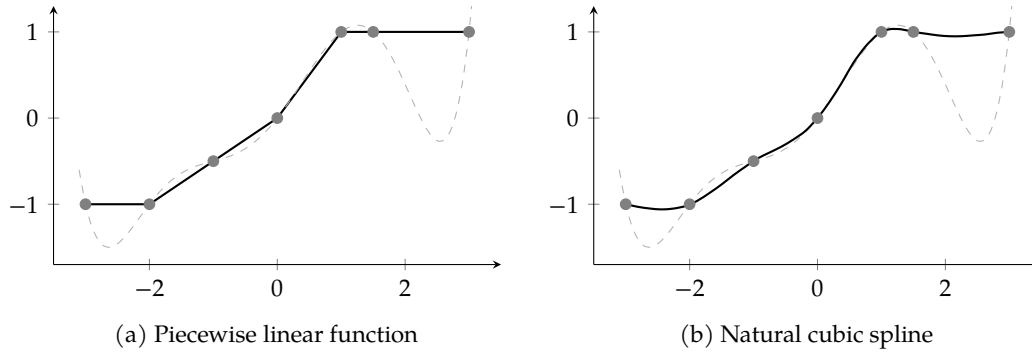


Figure 4.3: Spline interpolation of the points in fig. 4.2. The dashed line is the interpolation polynomial of degree six. Left: A piecewise linear function (spline of degree 1). Right: The natural cubic spline.

exists and it is continuous.<sup>5</sup> Assuming  $x_1 < \dots < x_n$ , we therefore have these conditions on the polynomial pieces  $p_i$  over the intervals  $[x_i, x_{i+1}]$ :

$$\begin{aligned}
 p_i(x_i) &= y_i & \text{for all } 1 \leq i \leq n-1 \\
 p_{n-1}(x_n) &= y_n \\
 p_i(x_{i+1}) &= p_{i+1}(x_{i+1}) & \text{for all } 1 \leq i \leq n-2 \\
 p'_i(x_{i+1}) &= p'_{i+1}(x_{i+1}) & \text{for all } 1 \leq i \leq n-2 \\
 p''_i(x_{i+1}) &= p''_{i+1}(x_{i+1}) & \text{for all } 1 \leq i \leq n-2
 \end{aligned}$$

The first two equations establish the interpolation property. The next three equations establish  $C^0$ -,  $C^1$ -, and  $C^2$ -continuity, respectively. Altogether we have  $4n - 6$  equations (conditions) but  $4n - 4$  coefficients (degrees of freedom) of the  $n - 1$  polynomials. This leaves us with two more conditions that we can impose:

- One common choice is to add  $p''_1(x_1) = p''_{n-1}(x_n) = 0$ . A cubic spline of this form is called *natural spline*.

This might be an attractive choice for the example of cam profiles, because this means that we start and end with zero acceleration.

- Another common choice is to add  $p'_1(x_1) = p'_{n-1}(x_n)$  and  $p''_1(x_1) = p''_{n-1}(x_n)$ . We can therefore plug copies of the splines together end-to-end and the result is still  $C^2$ -continuous. If in addition  $y_1 = y_n$  then the result is a periodic  $C^2$ -continuous function.

This choice is also attractive for cam profiles as we can periodically repeat the cam profile without jumps in acceleration (or velocity).

Figure 4.3b illustrates a natural cubic spline. Natural cubic splines have the nice property that they minimize strain energy: Consider a thin wooden strip that goes through the interpolation points. The wooden strip will take a form that minimizes the strain energy. The form that we get is exactly the one of the natural spline. This is essentially the reason why natural splines avoid the oscillating behavior of higher-degree interpolation polynomials.

<sup>5</sup>The set of  $k$ -times continuously differentiable functions is often denoted by  $C^k$ . We then also say that  $f$  is  $C^k$ -continuous. A  $C^0$ -continuous function means that  $f$  is simply continuous. In this sense a cubic spline is a  $C^2$ -continuous interpolating spline of degree three.

In order to compute a natural cubic spline we could simply solve the linear equation system formed by the  $4(n - 1)$  conditions. If we take a closer look, however, we see that this system can be significantly simplified and we end up with  $n - 1$  equations. Moreover, the simplified system actually has a special structure – it is in tridiagonal form – and can be solved in  $O(n)$  time by dedicated algorithms. Details can be found in appendix A.1.

Software packages like `scipy` for Python or `MATLAB` provide library functions that implement cubic spline computation. The following lines are from a Python interpreter shell and produced the data for fig. 4.3b:

```
>>> import scipy.interpolate as interp
>>> xs = [-3, -2, -1, 0, 1, 1.5, 3]
>>> ys = [-1, -1, -0.5, 0, 1, 1, 1]
>>> f = interp.CubicSpline(x, y, bc_type='natural')
>>> for x in np.linspace(-3, 3, 33):
...     print("{}, {}".format(x.round(2), f(x).round(2)))
...
(-3.0, -1.0)
(-2.81, -1.03)
[...]
(3.0, 1.0)
```

## 4.5 Numerical derivatives

Let  $f$  be a differentiable function. We would like to numerically compute  $f'(x)$  for some position  $x$ . Polynomials are easy to derive, so we could consider an interpolation polynomial  $p$  around  $x$  and take  $p'(x)$  instead. Maybe  $f$  is actually given in tabulated form so we cannot symbolically derive it anyway, but we can compute the interpolation polynomial.

This raises the question whether it is justified to take  $p'(x)$  as an approximation for  $f'(x)$ . Let us denote by  $x_1 < \dots < x_n$  the interpolation nodes. Recall eq. (4.4), which said that for any  $x$  there is a  $\xi$  such that

$$f(x) = p(x) + \frac{f^{(n)}(\xi(x))}{n!} \cdot w(x).$$

We explicitly write  $\xi(x)$  to emphasize that  $\xi$  depends on  $x$ . Assuming that  $\xi$  is differentiable, it is easy to show<sup>6</sup> that at all interpolation nodes  $x_k$  the following holds:<sup>7</sup>

$$f'(x_k) = p'(x_k) + \frac{f^{(n)}(\xi(x_k))}{n!} \cdot w'(x_k).$$

Note that  $w(x_k) = 0$  but  $w'(x_k)$  is not zero.<sup>8</sup> In other words,  $p'$  only *approximates*  $f'$  at interpolation nodes  $x_k$ , while  $p$  meets  $f$  exactly. Also note that if  $n = 1$  then  $p'(x) = 0$  so only  $n \geq 2$  is meaningful.

**Two-point formula.** In the simplest case we use  $n = 2$  interpolation nodes and therefore receive an interpolation polynomial of degree 1. Following eq. (4.12) and setting  $h = x_2 - x_1$  we

<sup>6</sup> $f'(x) = p'(x) + \frac{1}{n!}(f^{(n+1)}(\xi(x))\xi'(x)w(x) + f^{(n)}(\xi(x))w'(x))$  and  $w(x_k) = 0$ .

<sup>7</sup>The equation can also be proven without the assumption that  $\xi$  would be differentiable, but this is much harder.

<sup>8</sup>If  $w'(x_k) = 0$  would hold then  $w$  would have two roots at  $x_k$ , and hence two interpolation nodes would be equal.

have

$$p(x) = \frac{(x_2 - x)y_1 + (x - x_1)y_2}{h}$$

This immediately yields the so-called *two-point formula*

$$f'(x) \approx p'(x) = \frac{y_2 - y_1}{h} \quad (4.13)$$

Note that  $p'(x)$  does not depend on  $x$  anymore; it is constant. For any position  $x$  we approximate  $f'(x)$  by the slope of the secant formed by the interpolation nodes. In other words, we approximate the differential quotient by the difference quotient, see fig. 4.4a.

**Three-point formula.** Let us increase the number of nodes to  $n = 3$ . For a fixed  $h > 0$  we choose three equidistant interpolation nodes  $x_1 = x_2 - h, x_2, x_3 = x_2 + h$ . According to Lagrange's formula eq. (4.8) we have

$$p(x) = y_1 L_1(x) + y_2 L_2(x) + y_3 L_3(x) \quad \text{with} \quad L_k(x) = \prod_{\substack{i=1 \\ i \neq k}}^3 \frac{x - x_i}{x_k - x_i}$$

and therefore

$$p'(x) = y_1 L_1'(x) + y_2 L_2'(x) + y_3 L_3'(x). \quad (4.14)$$

Let us compute:

$$\begin{aligned} L_1(x) &= \frac{x - x_2}{-h} \cdot \frac{x - x_3}{-2h}, & L_1'(x) &= \frac{(x - x_2) + (x - x_3)}{2h^2} \\ L_2(x) &= \frac{x - x_1}{h} \cdot \frac{x - x_3}{-h}, & L_2'(x) &= \frac{(x - x_1) + (x - x_3)}{-h^2} \\ L_3(x) &= \frac{x - x_2}{h} \cdot \frac{x - x_1}{2h}, & L_3'(x) &= \frac{(x - x_1) + (x - x_2)}{2h^2} \end{aligned}$$

In order to compute  $f'$  at the middle node  $x_2$  we obtain the so-called *central three-point formula*:

$$f'(x_2) \approx p'(x_2) = \frac{y_1 \cdot (-h) + y_3 \cdot h}{2h^2} = \frac{y_3 - y_1}{2h}. \quad (4.15)$$

Note that  $L_2'(x_2) = 0$ , so  $y_2$  does not play a role anymore in the central three-point formula! In fact eq. (4.15) looks quite like eq. (4.13) for a simple reason: The central three-point formula gives the slope of the secant between the node  $x_1$  and  $x_3$ , see fig. 4.4b. Still,  $f'(x_2)$  is much better approximated using the central three-point formula than the two-point formula, because  $x_2$  sits in the middle between  $x_1$  and  $x_3$ . More precisely, in fig. 4.4b we obtain the tangent at  $x_2$  of the parabola through the three nodes.

However, if we are given  $f$  in a tabulated form and we want to compute  $f'$  at the first or last position then we cannot use the *central* three-point formula. But instead of resorting to the two-point formula, we can still receive a better result using eq. (4.14), but we plug in the left resp. right node:

$$f'(x_1) \approx p'(x_1) = y_1 \frac{-3h}{2h^2} + y_2 \frac{-2h}{-h^2} + y_3 \frac{-h}{2h^2} = \frac{-3y_1 + 4y_2 - y_3}{2h}$$

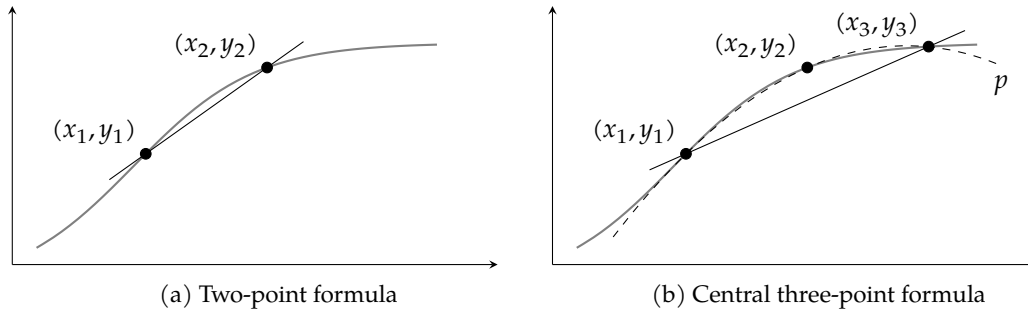


Figure 4.4: Numerical derivative of  $\tanh(x)$  using interpolation polynomials  $p$  with two (left) and three (right) nodes.

## 4.6 Numerical integration

We start with a similar situation as for numerical differentiation: Let  $f: [a, b] \rightarrow \mathbb{R}$  be the function to be integrated. We replace  $f$  by a polynomial  $p$  and consider the integral of  $p$  over  $[a, b]$  instead. However, while computing  $f'(x)$  is a local problem at the position  $x$ , in order to integrate  $f$ , we have to consider  $f$  globally on  $[a, b]$ .

Remember that we learned two approaches for a polynomial interpolation of  $f$  in this chapter: A single polynomial or a spline. In the first case we obtain the basic integration formulas in section 4.6.1 and in the second case we obtain extended formulas section 4.6.2.

### 4.6.1 Basic integration formulas

Our goal is to numerically compute the integral of a function  $f$  over an interval  $[a, b]$ . We choose  $n + 1$  equidistant nodes

$$x_k = a + k \cdot h,$$

where  $0 \leq k \leq n$  and  $h = (b-a)/n$  is called the step size. Similar to numerical derivatives, we compute an interpolation polynomial  $p$  for  $f$ , which we can integrate. We set

$$y_k = f(x_k).$$

Using Lagrange's formula from eq. (4.8) we obtain

$$\int_a^b f(x) \, dx \approx \int_a^b p(x) \, dx = \sum_{k=0}^n y_k \int_a^b L_k(x) \, dx.$$

Hence, the entire problem of numerical integration is essentially reduced to computing the terms

$$A_k = \int_a^b L_k(x) \, dx. \quad (4.16)$$

We can simplify a bit more by transforming the interval  $[a, b]$  to  $[0, n]$  via a transformation

$$t = \frac{x-a}{h} \quad \text{resp.} \quad x = a + th.$$

Applying this transformation to the definition of  $L_k(x)$  in eq. (4.9) we obtain

$$L_k(x) = \prod_{\substack{i=0 \\ i \neq k}}^n \frac{x - x_i}{x_k - x_i} = \prod_{\substack{i=0 \\ i \neq k}}^n \frac{t - i}{k - i}.$$

Applying this transformation to eq. (4.16) we then get

$$A_k = \int_a^b L_k(x) \, dx = h \int_0^n L_k(x) \, dt = h \int_0^n \prod_{\substack{i=1 \\ i \neq k}}^n \frac{t - i}{k - i} \, dt.$$

With

$$\alpha_k^{(n)} = \int_0^n \prod_{\substack{i=1 \\ i \neq k}}^n \frac{t - i}{k - i} \, dt \quad (4.17)$$

we have

$$A_k = h \alpha_k^{(n)}.$$

This now gives us the so-called (*closed*) *Newton-Cotes formula*<sup>9</sup> of degree  $n$ :

$$\int_a^b f(x) \, dx \approx h \sum_{k=0}^n f(x_k) \alpha_k^{(n)}. \quad (4.18)$$

All that remains is to make a choice about  $n$  and to compute  $\alpha_0^{(n)}, \dots, \alpha_n^{(n)}$ . Different choices of  $n$  then give us different *integration rules*, e.g., the Trapezoidal rule, Simpson's rule, Simpson's 3/8 rule, Boole's rule for  $n = 0, 1, 2, 3$ , respectively. In the following, we compute the first two examples.

**Trapezoidal rule.** We start with the case  $n = 1$  and solve eq. (4.17):

$$\begin{aligned} \alpha_0^{(1)} &= \int_0^1 \frac{t - 1}{0 - 1} \, dt = \frac{1}{2} \\ \alpha_1^{(1)} &= \int_0^1 \frac{t - 0}{1 - 0} \, dt = \frac{1}{2} \end{aligned}$$

Plugging the results in eq. (4.18) gives the *trapezoidal rule*:

$$\int_a^b f(x) \, dx \approx h \frac{f(a) + f(b)}{2} \quad (4.19)$$

We can interpret this rule as replacing  $f$  by a single linear function interpolating at  $a$  and  $b$ , whose integral corresponds to the area of the resulting trapezoid.

**Simpson's rule.** Increasing the number of nodes to  $n = 2$  we obtain after some calculations

$$\alpha_0^{(2)} = \frac{1}{3} \quad \alpha_1^{(2)} = \frac{4}{3} \quad \alpha_2^{(2)} = \frac{1}{3}.$$

The resulting formula is known as *Simpson's rule* or *Simpson's 1/3 rule* or *Kepler's barrel rule*:

$$\int_a^b f(x) \, dx \approx \frac{h}{3} \left( f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right). \quad (4.20)$$

---

<sup>9</sup>We can apply the very same procedure without including the boundary points  $a$  and  $b$  as interpolation nodes. This then yields the open Newton-Cotes formulas.

## 4.6.2 Extended formulas

Applying the Newton-Cotes formulas for higher degree maneuvers ourselves into the problem of Runge's phenomenon. Hence, instead of determining the  $\alpha_k^{(n)}$  for large  $n$ , we actually use the simpler Trapezoidal or Simpson rule, but apply it on sub-intervals of  $[a, b]$ . This then yields the *extended Newton-Cotes formulas* or *composite rules*.

We start with dividing  $[a, b]$  into  $N$  parts of equal length

$$H = \frac{b - a}{N}.$$

Each part is now a sub-interval  $[z_{j-1}, z_j]$  with

$$z_j = a + jH$$

and we compute

$$\int_a^b f(x) \, dx = \sum_{j=1}^N \underbrace{\int_{z_{j-1}}^{z_j} f(x) \, dx}_{I_j}.$$

Using the trapezoidal rule for  $I_j$  gives the *extended trapezoidal rule*:

$$\int_a^b f(x) \, dx \approx \frac{H}{2} \left( f(z_0) + f(z_N) + 2 \sum_{j=1}^{N-1} f(z_j) \right).$$

Using the Simpson's rule for  $I_j$  gives the *extended Simpson's rule* and therefore we use  $2N + 1$  nodes for  $N$  intervals and have  $h = H/2$  in eq. (4.20). We denote the nodes as  $x_j = a + j\frac{H}{2}$  for  $0 \leq j \leq 2N$  and obtain

$$\begin{aligned} \int_a^b f(x) \, dx &\approx \frac{h}{3} \left( f(x_0) + f(x_{2N}) + 2 \sum_{k=1}^{N-1} f(x_{2k}) + 4 \sum_{k=1}^{N-1} f(x_{2k-1}) \right) \\ &= \frac{H}{6} (f(x_0) + 4f(x_1) + 2f(x_2) + 4f(x_3) + 2f(x_4) + \cdots + f(x_{2N})). \end{aligned}$$

## 4.7 Richardson extrapolation

Assume that we compute a numerical integral with a step size  $h$ . Then we can compute the numerical integral for smaller and smaller step sizes and extrapolate the case where the step size  $h$  would become zero in the limit. This is a very useful general idea that goes by *Richardson extrapolation*. Richardson extrapolation is therefore a method to accelerate convergence of a sequence. A well known application is *Romberg integration*.

### 4.7.1 Limit of a sequence

Polynomial interpolation is typically not well suited for extrapolation, i.e., for the computation of  $f(x)$  when  $x$  is outside the interval of the interpolation nodes. However, one exception is when the nodes  $x_1, \dots, x_n$  form the prefix of a sequence  $(x_i)$  that converges against  $x$ .



Let us consider a function  $f$  and we would like to extrapolate  $f(0)$ . With a fixed  $h > 0$  we choose nodes

$$x_i = \frac{h}{2^{i-1}}.$$

The sequence  $(x_i) = (h, h/2, h/4, \dots)$  converges to zero. The Neville recursion in eq. (4.11) for  $f(0) = T_{1,\dots,n}$  now becomes a bit simpler:

$$T_i = f(x_i)$$

$$T_{i,\dots,i+m} = \frac{2^m T_{i+1,\dots,i+m} - T_{i,\dots,i+m-1}}{2^m - 1}.$$

For certain applications, such as Romberg integration, it may turn out that  $f$  is an even function, which means  $f(x) = f(-x)$ . In this case we would also use an even polynomial function  $p(x) = a_0 + a_2x^2 + a_4x^4 + \dots$  for extrapolation, where the odd terms  $x, x^3, \dots$  are removed. Then we can actually substitute  $t = x^2$ , which gives  $p(t) = a_0 + a_2t + a_4t^2 + \dots$  and nodes  $t_i = x_i^2 = h^2/4^{i-1}$ . This leads finally to an improved Neville recursion

$$T_i = f(t_i) \tag{4.21}$$

$$T_{i,\dots,i+m} = \frac{4^m T_{i+1,\dots,i+m} - T_{i,\dots,i+m-1}}{4^m - 1}. \tag{4.22}$$

### 4.7.2 Romberg integration

Romberg integration is Richardson extrapolation applied to the extended trapezoidal rule for numerical integration. That is, we consider

$$T(h) = \frac{h}{2} \left( f(x_0) + f(x_N) + 2 \sum_{j=1}^{N-1} f(x_j) \right).$$

for  $x_j = a + jh$  and  $h = (b-a)/N$ . Then it holds that

$$\lim_{h \rightarrow 0} T(h) = \int_a^b f(x) \, dx.$$

It now turns out that the Taylor series of  $T$  actually only consists of even powers<sup>10</sup> and hence  $T$  is an even function. This now allows us to apply eq. (4.22) to extrapolate  $T(0)$ . This method is known as the *Romberg integration*.

---

<sup>10</sup>This is a consequence of the Euler-Maclaurin formula.



**Part III**

**Computational Geometry**



# Geometric computations

## 5.1 Introduction

Many algorithmic problems in industrial application domains – GIS<sup>1</sup>, computer graphics, CAD/-CAM<sup>2</sup> and robotics, logistics, drug exploration in pharmacy, et cetera – have a strong geometric flavor. For instance, computing the shortest path for a car on a street map, routing a wire on a PCB<sup>3</sup>, computing offset paths for CNC machining, intersecting geometric shapes in a graphics design software, shooting and intersecting a ray with objects in a 3D scenery.

The field of *computational geometry* is about algorithms and data structures in a geometric context. Devising algorithms and analyzing their computational efficiency concerning time and space is the dominant part in this research field. From a practical point of view, however, algorithm engineering in computational geometry also needs to address computing with geometric objects – like points and lines – just like we did for numbers in chapter 2.

A large number of topics in computational geometry are actually of strong combinatorial nature, and this field is aptly called *combinatorial geometry*. Take for instance the street network of Austria on which we would like to compute shortest routes. From an initial point of view this is evidently a geometric problem. But at second glance, we can forget about the precise coordinates of cities and junctions and observe that the problem is actually driven by a semi-geometrical network structure: by the “topology” of the street network (combinatorial structure) which tells which street sections interconnect the network nodes and the length of these street sections (geometric structure). This is why computational geometry is closely related to combinatorics, topology and graph theory.<sup>4</sup>

## 5.2 Geometric constructions and predicates

A *predicate* is a boolean property of objects. For instance, the predicate  $f: \mathbb{Z} \rightarrow \{\text{false}, \text{true}\}: f(x) \bmod 2 = 0$  on the set of whole numbers tells whether a number is even. A geometric example would be a predicate on the set of pair of lines telling whether the pair would intersect. Another predicate given a circle and a point would be whether the point lies within the circle.

Unlike a predicate, a geometric *construction* produces geometric objects, like points or lines. So while a predicate asks whether two lines intersect, a geometric construction would compute

<sup>1</sup>Geographic Information Systems

<sup>2</sup>Computer-Aided Design, Computer-Aided Manufacturing

<sup>3</sup>Printed-circuit board

<sup>4</sup>There is also a smaller subfield of “geometry of numbers” within discrete and combinatorial geometry, which is part of number theory. There is a tradition in Vienna towards this field, see for instance the subspace theorem by Schmidt.

the actual intersection point of two lines, or the circumcenter of a triangle, or the line between two points.

Many geometric algorithms require no constructions but require predicates only. For instance, given a finite point set  $\{p_1, \dots, p_n\} \in \mathbb{R}^2$  then we compute the convex hull (see chapter 6) using predicates only. Indeed the geometric predicate telling whether a point lies left to a ray is all we need.

### 5.2.1 Construction of orthogonal vectors

A simple example for a construction is the rotation of a vector by the angle  $\varphi = 90^\circ$ . This is achieved by simply switching coordinates and changing sign of one coordinate:

$$\begin{pmatrix} x \\ y \end{pmatrix} \cdot \begin{pmatrix} -y \\ x \end{pmatrix} = xy - yx = 0. \quad (5.1)$$

The vectors are orthogonal as the inner product is zero. For a rotation by  $90^\circ$  we have two ways to switch sign; the one rotates in counterclockwise direction, the other in clockwise direction. This is also evident from the rotation matrix by a counterclockwise angle  $\varphi$ :

$$\begin{pmatrix} \cos \varphi & -\sin \varphi \\ \sin \varphi & \cos \varphi \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 0 & -1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} -y \\ x \end{pmatrix}$$

So a rotation by  $90^\circ$  can be done very quickly *without* loss in numerical precision and computationally fast as well. This is important because basic geometric predicates can be implemented using right-angle rotations of vectors.

### 5.2.2 Orientation of three points

We will later learn about the Graham scan algorithm for convex hulls, see algorithm 4. If we look carefully then all we need for this algorithm from a geometric perspective is the test – the predicate – whether three points form a left turn. This is the only numerical part.

Actually, there are many ways to phrase this question, see fig. 5.1. Given three points  $p, q, r \in \mathbb{R}^2$ , we may ask whether the triangle  $pqr$  is oriented counterclockwise, or whether  $r$  is left to the ray  $\overrightarrow{pq}$ , or whether the polygonal chain  $pqr$  forms a left turn.

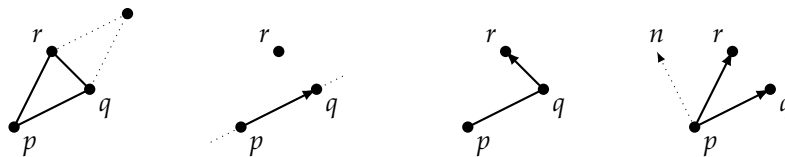


Figure 5.1: Four formulations of the same question: Is triangle  $pqr$  ccw oriented, is  $r$  left to  $\overrightarrow{pq}$ , is the polygonal chain  $pqr$  a left turn, and is the rotation of  $\overrightarrow{pq}$  to  $\overrightarrow{pr}$  less than a half turn? All are answered by  $\Delta(p, q, r) > 0$ .

A *bad* idea would be to actually compute and compare the angles of the vectors  $\overrightarrow{pq}$  and  $\overrightarrow{pr}$ , because this involves trigonometric functions, which are in general inaccurate and slow. Let us instead consider the parallelogram formed by the vectors  $\overrightarrow{pq}$  and  $\overrightarrow{pr}$  in the left figure of fig. 5.1.

There is a formula for the *signed* area of this parallelogram given by the following determinant:

$$\Delta(p, q, r) = \begin{vmatrix} p_x & q_x & r_x \\ p_y & q_y & r_y \\ 1 & 1 & 1 \end{vmatrix} = p_x q_y + q_x r_y + r_x p_y - p_x r_y - q_x p_y - r_x q_y. \quad (5.2)$$

By “signed area” we mean that  $|\Delta(p, q, r)|$  is the area, but  $\Delta(p, q, r)$  is positive if  $pqr$  is counterclockwise (ccw) oriented, negative if  $pqr$  is clockwise (cw) oriented and zero if  $p, q, r$  are collinear<sup>5</sup>. In other words,  $\Delta(p, q, r)$  is twice the signed area of the triangle  $pqr$ . The matrix in eq. (5.2) is actually related to homogeneous coordinates, which are heavily used in computer graphics and robotics.<sup>6</sup>

The last figure in eq. (5.2) is somewhat different in the sense that it compares the two vectors  $q - p$  and  $r - p$  rather than three points. Let us denote by  $n$  the vector we obtain by rotating the vector  $q - p$  by  $90^\circ$  in ccw direction. We then ask whether  $r - p$  projected onto  $n$  is positive, i.e., whether the inner product  $n \cdot (r - p)$  is positive. Note that  $n = (-(q_y - p_y), (q_x - p_x))$  by eq. (5.1) and hence

$$n \cdot (r - p) = \begin{pmatrix} -(q_y - p_y) \\ q_x - p_x \end{pmatrix} \cdot \begin{pmatrix} r_x - p_x \\ r_y - p_y \end{pmatrix} = (q_x - p_x) \cdot (r_y - p_y) - (q_y - p_y)(r_x - p_x) \quad (5.3)$$

On the other hand

$$\Delta(p, q, r) = \begin{vmatrix} p_x & q_x & r_x \\ p_y & q_y & r_y \\ 1 & 1 & 1 \end{vmatrix} = \begin{vmatrix} p_x & q_x - p_x & r_x - p_x \\ p_y & q_y - p_y & r_y - p_y \\ 1 & 0 & 0 \end{vmatrix} = (q_x - p_x) \cdot (r_y - p_y) - (q_y - p_y)(r_x - p_x)$$

and so we just learned that  $\Delta(p, q, r) = n \cdot (r - p)$ .<sup>7</sup> Note that eq. (5.3) only requires two multiplications, but at the expense of a numerical asymmetry as  $p_x$  and  $p_y$  are occurring twice.

---

**Algorithm 1** An algorithm that tests whether the points  $pqr$  are in ccw orientation.

---

```

procedure ccw( $p, q, r$ )
  return  $p_x q_y + q_x r_y + r_x p_y - p_x r_y - q_x p_y - r_x q_y$ 
end procedure

```

---

We can summarize these insights in algorithm 1. Note that we deliberately do not return a boolean value but a numerical value for two reasons: First, we can distinguish three cases: ccw, collinear, cw. Secondly, the comparison against zero requires in general some epsilon threshold and the epsilon is application dependent, so we leave it to the caller.

### 5.2.3 Point location in triangles and convex polygons

Assume we are given a convex polygon  $P = (p_1, \dots, p_n)$  with its vertices  $p_i$  given in ccw order, as illustrated in fig. 5.2. (We learn about convexity in section 6.1, but for now it suffices to know that a convex polygon has no dents.) We would like to test whether a given point  $r$  is in  $P$  or not. In particular,  $P$  could be a triangle.

---

<sup>5</sup>Collinear means that they reside on a common line.

<sup>6</sup>The idea behind homogeneous coordinates is to embed the plane  $\mathbb{R}^2$  into three space as  $\mathbb{R}^2 \times \{1\}$  by setting the z-coordinate of all points to 1. By this trick the translation of points becomes a linear operation. The vectors  $p, q, r$  span a basis of  $\mathbb{R}^3$ , if not collinear, and the sign of  $\Delta(p, q, r)$  tells us the orientation of the basis. Moreover,  $\Delta(p, q, r)$  gives us the signed volume of the “unit cube” in this basis, i.e., the signed volume of  $\{\lambda_1 p + \lambda_2 q + \lambda_3 r : \lambda_i \in [0, 1]\}$ . The plane  $\mathbb{R}^2 \times \{1\}$  can also be interpreted as the two-dimensional projective plane.

<sup>7</sup>And now we directly see that  $\Delta(p, q, r)$  is the signed area of the parallelogram of the left figure in fig. 5.1.

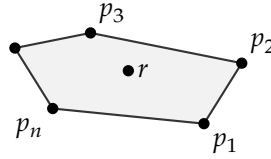


Figure 5.2: A point is in a convex polygon if it lies to the left of all edges in ccw direction.

The convexity of  $P$  makes this a very simple task as  $r$  is in  $P$  if and only if  $r$  lies to the left of all edges, i.e., to the left of all rays  $\overrightarrow{p_1p_2}, \overrightarrow{p_2p_3}, \dots, \overrightarrow{p_np_1}$ . In other words, if  $r$  lies outside of  $P$  then  $r$  lies to the right of some edge of  $P$ . So a simple algorithm that runs in  $O(n)$  time is the one given in algorithm 2.

---

**Algorithm 2** An algorithm that tests in linear time whether a point  $p$  is in a convex polygon  $P$  given in ccw direction.

---

```

procedure IN_CONVEX_CCW_POLYGON( $P, r$ )
  for  $i \in \{1, \dots, n\}$  do
    if  $\text{CCW}(p_i, p_{1+(i \bmod n)}, r) < 0$  then
      return false
  return true
end procedure

```

---

If, however,  $P$  would not have been convex then a reasonably simple solution could be to triangulate the polygon and make the test for every triangle. There are, however, more efficient methods.

## 5.2.4 Intersection of two line segments

Given two line segments  $\overline{ab}$  and  $\overline{cd}$ , we can use the predicate  $\text{ccw}$  alone to test whether the two line segments intersect. All we have to do is to check that the endpoints of  $\overline{cd}$  lie on different sides of  $\overline{ab}$ , and vice versa. So four invocations of  $\text{ccw}$  are sufficient. (Note that testing it vice versa is necessary!)

## 5.2.5 Point location in circle

Given a circle and a point  $p \in \mathbb{R}^2$ , we can ask whether the point is within, on, or outside the circle. Depending on how the circle is given, the answers are more or less trivial.

In the simple case the circle is given by a center point  $c \in \mathbb{R}^2$  and a radius  $r \geq 0$ . Then we simply check whether the distance of  $p$  to  $c$  is less, equal or greater to  $r$ , i.e., we compare  $\|p - c\|$  against  $r$ . For numerical and efficiency reasons we of course avoid square roots when computing distances between points and instead compare squared distances as a general rule of thumb:

$$(p_x - c_x)^2 + (p_y - c_y)^2 \leq r^2 \quad (5.4)$$

In the more involved case the circle is given by three points  $a, b, c \in \mathbb{R}^2$ . In other words, the circle is given as the circumcircle of the triangle  $abc$ . We assume that  $a, b, c$  are given in



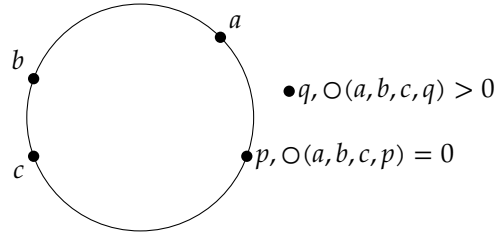


Figure 5.3: Illustration of the in-circle point location test for a circle spanned by three points.

counterclockwise direction – we know already how to check – then we can test the sign of the following determinant

$$\mathcal{O}(a, b, c, p) = \begin{vmatrix} a_x & a_y & a_x^2 + a_y^2 & 1 \\ b_x & b_y & b_x^2 + b_y^2 & 1 \\ c_x & c_y & c_x^2 + c_y^2 & 1 \\ p_x & p_y & p_x^2 + p_y^2 & 1 \end{vmatrix}. \quad (5.5)$$

If  $\mathcal{O}(a, b, c, p)$  equals zero then  $p$  is on the circle, if it is negative then  $p$  is within the circle and if it is positive then  $p$  is outside the circle. Note that no square roots are required here. A proof sketch behind this can be found in appendix A.2.



# Convex hull

## 6.1 Convexity

Convex hulls are a very basic concept in the field of computational geometry and often used as a preprocessing step for other algorithms. Assume we are given  $n$  points in the plane that vaguely resemble a shape in the plane, as in fig. 6.3. How do we restore the shape in terms of a polygon? One answer to this could be the *convex hull*.<sup>1</sup> Let us first introduce a few definitions.

**Definition 1.** We call a set  $A \subseteq \mathbb{R}^d$  *convex* if for any two points  $p, q \in A$  the entire line segment  $\overline{pq}$  is contained in  $A$ .

In fig. 6.1 we illustrate two sets in  $\mathbb{R}^2$ . The right set is non-convex because we can find two points  $p$  and  $q$  such the line segment  $\overline{pq}$  is not entirely contained in  $A$ . So vaguely speaking, a set is convex if it has no “embayment” like the one in fig. 6.1b. As a general rule of thumb in mathematics and computer science, we can say that problems tend to become simpler if they are convex. Take for instance the predicate whether a point is in a (convex) polygon in section 5.2.3.<sup>2</sup>

So far, we did not say how we exactly define  $\overline{pq}$ . Since  $\mathbb{R}^d$  is a vector space we can define

$$\overline{pq} = \{\lambda p + (1 - \lambda)q : \lambda \in [0, 1]\}.$$

where we see  $p$  and  $q$  as vectors. This is a convenient definition from an algorithmic point of view, as we can simply *compute* all points on the line segment  $\overline{pq}$  by choosing a  $\lambda \in [0, 1]$  and computing the vector  $\lambda p + (1 - \lambda)q$ . We get the endpoint  $q$  for  $\lambda = 0$ , the endpoint  $p$  for  $\lambda = 1$  and all points in between for  $0 < \lambda < 1$ . For instance, we get the mid point of  $\overline{pq}$  for  $\lambda = \frac{1}{2}$ . The expression  $\lambda p + (1 - \lambda)q$  with  $0 \leq \lambda \leq 1$  is called a *convex combination* of  $p$  and  $q$ , which is a special case of a linear combination. More generally, for points (or vectors)  $p_1, \dots, p_n$  we call the linear combination

$$\lambda_1 p_1 + \lambda_2 p_2 + \dots + \lambda_n p_n$$

a *convex combination* if  $\sum_{i=1}^n \lambda_i = 1$  and  $\lambda_i \in [0, 1]$  for all  $0 \leq i \leq n$ . The set of convex combinations of two points  $p$  and  $q$  is the line segment  $\overline{pq}$  and the set of convex combinations of three points  $p, q, r$  is the triangle formed by the three points. If we set the coefficients  $\lambda_i$  all equal to  $1/n$  then we obtain the *center of gravity*, see fig. 6.2.

<sup>1</sup>For non-convex shapes the so-called *alpha shape* is a generalization of the convex hull that can be used for this shape restoration task.

<sup>2</sup>Personal remark: Peter Gruber used to say that if mathematical functions and bodies have certain properties then convexity often makes these properties even stronger, see also [12, p. VI]. In this sense, *convexity* is the steroids of mathematical properties, which eventually also makes algorithms simpler and more powerful.

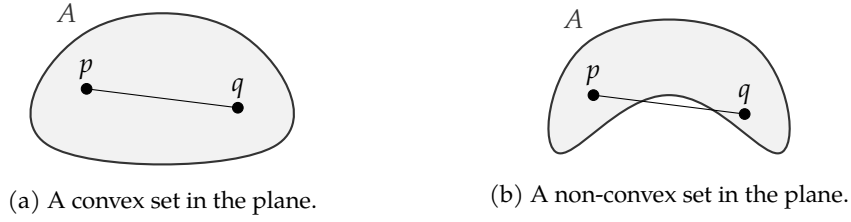


Figure 6.1: A set  $A$  is called convex if for each pair of points  $p, q \in A$  the entire line segment  $\overline{pq}$  is contained in  $A$ .

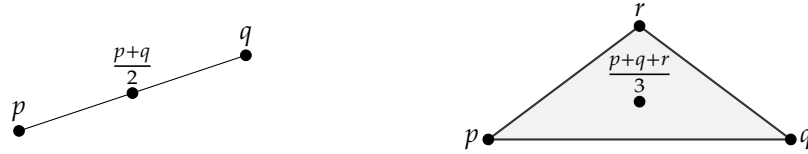


Figure 6.2: The set of convex combinations of two points forms a line segment. The set of convex combinations of three points forms a triangle. By setting the coefficients all equal we obtain the center of gravity, e.g.,  $(p+q)/2$  for the line segment and  $(p+q+r)/3$  for the triangle.

**Definition 2.** We define the *convex hull*  $\text{conv}\{p_1, \dots, p_n\}$  of  $n$  points  $p_1, \dots, p_n \in \mathbb{R}^d$  as the smallest<sup>3</sup> convex set that contains  $p_1, \dots, p_n$ . More generally, for a set  $A \subseteq \mathbb{R}^d$  we define  $\text{conv } A$  as the smallest convex superset of  $A$  in  $\mathbb{R}^d$ .

Let us consider the finite point set  $p_1, \dots, p_n$  in fig. 6.3. By definition  $\text{conv}\{p_1, \dots, p_n\}$  is the smallest convex superset of  $\{p_1, \dots, p_n\}$ . However, it is also the set of all convex combinations of  $p_1, \dots, p_n$ . In other words, in fig. 6.2 the line segment is equal  $\text{conv}\{p, q\}$  and the triangle is equal  $\text{conv}\{p, q, r\}$ . The convex hull of a finite point set in the plane is a convex polygon and the convex hull of a finite point set in higher-dimensional space is a convex polyhedron.

An intuitive visualization of the *smallest* convex super set in the plane is the following: We place at each point  $p_i$  a nail and put a tight elastic rubber band around the point set. When the rubber band shrinks it attains the shape of  $\text{conv}\{p_1, \dots, p_n\}$  as in fig. 6.3.

Adding or removing a nail (point) in the interior does not change the rubber band (convex hull). In particular, adding *any* convex combination of  $p_1, \dots, p_n$  to the point set does not change the convex hull. This is a nice insight we can use to speed-up algorithms for convex hulls by reducing the number of input points: We take any three input points from fig. 6.3, form a triangle, and any input point in (the interior of) this triangle can be discarded.<sup>4</sup>

## 6.2 Quickhull

Discarding points in triangles leads us directly to the divide-and-conquer convex hull algorithm *quickhull*, whose name is derived from the quicksort algorithm [3]. The quickhull algorithm is implemented in the well known qhull [2] software library.

<sup>3</sup>“smaller” than  $B$  if  $A \subseteq B$ . However, it is actually not immediately clear why there would only one smallest convex super set as  $\subseteq$  does not yield a total order. Hence, the convex hull may instead be defined as the infinite intersection of all convex supersets and then it is shown that the result is (i) convex and (ii) the smallest such set.

<sup>4</sup>A more practical variant is to remove all points of large axis-aligned rectangles instead of triangles, see [13].

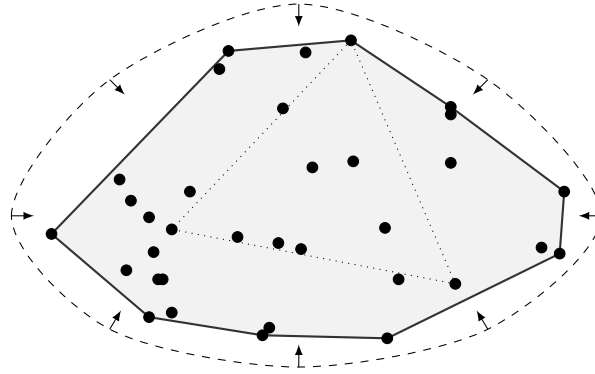


Figure 6.3: The convex hull of  $n$  input points in the plane forms a convex polygon. We can think of it as the resulting shape of a tight elastic rubber band (dashed line) around nails placed at the input points. Any triangle (dotted) formed by three input points is entirely contained in the convex hull.

**The algorithm.** The quickhull algorithm separately computes the upper and the lower part of the convex hull by repeatedly discarding points in triangles. It starts by finding the left-most point  $p$  and the right-most point  $q$  of the point set, see fig. 6.4a. For the upper part it considers the point  $r$  with largest orthogonal distance to  $\overline{pq}$ , but to the left of the ray  $\overrightarrow{pq}$ . We learned that all points in the triangle  $pqr$  can be discarded.

Next it recursively repeats by constructing triangles and discarding points: It considers the line  $\overline{pr}$  and finds the point with largest orthogonal distance, again to the left of  $\overrightarrow{pr}$ . All points in there are discarded. Then it does the same for the ray  $\overrightarrow{rq}$ : It constructs a triangle with the point that is left-most to  $\overrightarrow{rq}$  and discards points, see fig. 6.4b. When no points are left it is done with the upper part. The entire algorithm is summarized in algorithm 3.

The essential idea can be generalized to convex hulls in  $\mathbb{R}^d$ . Instead of triangles we have simplices<sup>5</sup> of higher dimension, see [3] for details.

**Analysis.** Let us consider algorithm 3. If the  $n$  input points are distributed in an unfavorable way then  $O(n)$  many calls of PARTIALHULL cost  $O(n)$  time each, which leads to a total of  $O(n^2)$  time in the worst case. However, if the recursion is balanced well then the recursion depth is  $O(\log n)$  and on each recursion level we spend in total  $O(n)$  time, leading to total time complexity of  $O(n \log n)$ .

## 6.3 Graham scan

A simple algorithm that runs in  $O(n \log n)$  time in the worst case is Graham's scan. It essentially orders the points by angles around an anchor point and then iteratively constructs the hull. Here, however, we present a practical variant of the original algorithm that separately computes the upper and lower part of the convex hull and avoids sorting the points by angles, which would be unfavorable in terms of numerics and speed.

<sup>5</sup>A  $d$ -dimensional simplex, or  $d$ -simplex, is the convex hull of  $d + 1$  points in  $\mathbb{R}^d$ . It is a line segment in  $\mathbb{R}^1$ , a triangle in  $\mathbb{R}^2$ , a tetrahedron in  $\mathbb{R}^3$ .

```

procedure QUICKHULL( $S$ )
     $p \leftarrow \arg \min_{v \in S} v.x$ 
     $q \leftarrow \arg \max_{v \in S} v.x$ 
    return PARTIALHULL( $S, p, q$ ) + PARTIALHULL( $S, q, p$ )
end procedure

procedure PARTIALHULL( $S, p, q$ )
     $S \leftarrow \{v \in S : p, q, v \text{ is a left turn}\}$ 
    if  $|S| \leq 1$  then
        return  $[p] + S$ 
    end if
     $r \leftarrow \arg \max_{v \in S} d(v, \overrightarrow{pq})$ 
    return PARTIALHULL( $S, p, r$ ) + PARTIALHULL( $S, r, q$ )
end procedure

```

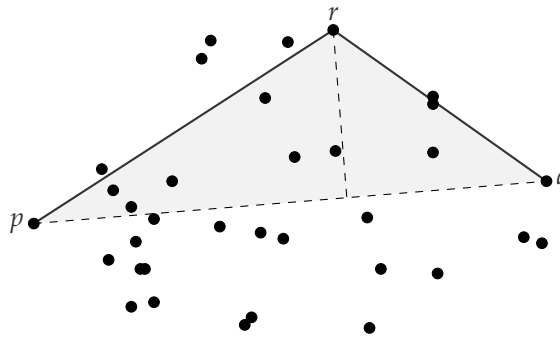


Figure 6.4: The quickhull algorithm separately computes the upper and the lower part of the convex hull. Here we only illustrate the upper part.

**Algorithm.** We start by sorting the points lexicographically, i.e., primarily by the  $x$ -coordinate and secondarily by the  $y$ -coordinate. The left-most point  $p$  and right-most point  $q$  are the first and last point in this order. To compute the upper convex hull in fig. 6.5 we first remove all points right to  $\overline{pq}$ . If we connect the remaining points we obtain a polygonal chain that starts at  $p$ , makes a zig-zag line to the right, and ends at  $q$ . The upper convex chain only contains right turns, so our goal is to remove all left turns.

In `PARTIALHULL` in algorithm 4 we compute the upper convex hull iteratively. Assume that our last two points in our result is  $r$  and  $u$  and we are about to add  $v$ . In fig. 6.5 the triple  $r, u, v$  forms a right turn, so we simply add  $v$ . Next we are about to add  $w$ , but  $u, v, w$  is a left turn, so we remove  $v$  again. Now we consider  $r, u, w$  which is still a left turn, so we remove  $u$ , too. Now we have  $p, r, w$  which is a right turn, and we proceed with the next vertex.

**Analysis.** The first step of `GRAHAMSCAN` is a sort operation, which takes  $O(n \log n)$  time. All the rest runs in  $O(n)$  time, including the double loop in `PARTIALHULL(.)`. The reason for the latter is the following counting argument: Each vertex  $v \in S$  is considered at most twice, because it is appended once and removed at most once. Hence, the `POPBACK` operation in the inner loop can only be executed  $O(n)$  times.

## 6.4 Lower bound on the time complexity

From the above analysis we learned that Graham scan is – from the perspective of time complexity – essentially sorting points. Interestingly, the opposite is also true: We can sort numbers using a convex hull algorithm. Assume we would like to sort the numbers  $x_1, \dots, x_n$ . We start by creating points  $p_i = (x_i, x_i^2)$  on a parabola. When we compute the convex hull with *any* algorithm then every point  $p_i$  is part of  $\text{conv}\{p_1, \dots, p_n\}$ , and we just read off the  $x_i$  in sorted order from the convex hull.

We know from algorithm theory that  $O(n \log n)$  is a lower bound for sorting  $n$  numbers.<sup>6</sup> Assume that there is a convex hull algorithm that is faster than  $O(n \log n)$ . Computing the points on the parabola, computing the convex hull, and reading off the points from the result is therefore also faster than  $O(n \log n)$ . Hence, we sorted numbers in time less than  $O(n \log n)$ , which is a contradiction.

We just proved that any convex hull algorithm takes at least as much time as sorting numbers, namely  $O(n \log n)$  time. We did so by reducing the problem of sorting to the problem of convex hulls, so a lower bound on sorting must also apply to computing convex hulls. This *reduction* technique is a general technique to derive lower bounds on the complexity of problems.

What we also showed is that the Graham scan algorithm is worst-case *time optimal* in the sense of asymptotic time complexity.

## 6.5 Applications

The convex hull is a basic tool in computational geometry. The reconstruction of a (convex) shape from a set of points is one immediate application, but often we use convex hulls as one step of other geometric algorithms. For instance, the convex hull can be exploited to compute

---

<sup>6</sup>There is no sorting algorithm based on key comparison that takes less than  $O(n \log n)$  time.

---

**Algorithm 4** The Graham scan algorithm to compute  $\text{conv } S$ .

---

<pre> <b>procedure</b> GRAHAMSCAN(<math>S</math>)   <math>S \leftarrow \text{SORT}(S)</math>   <math>p \leftarrow S[0]</math>   <math>q \leftarrow S[-1]</math>   <b>return</b> PARTIALHULL(<math>S, p, q</math>) + PARTIALHULL(REVERSE(<math>S</math>), <math>q, p</math>) <b>end procedure</b> </pre>	<p>▷ Compute convex hull of point set <math>S</math></p> <p>▷ Sort points lexicographically by <math>(x, y)</math></p> <p>▷ Left-most input point</p> <p>▷ Right-most input point</p>
<pre> <b>procedure</b> PARTIALHULL(<math>S, p, q</math>)   <math>S \leftarrow \{v \in S : p, q, v \text{ is a left turn}\}</math>   <math>H \leftarrow []</math>   <b>for</b> <math>v \in S</math> <b>do</b>     <b>while</b> <math> H  \geq 2</math> and <math>H[-2], H[-1], v</math> is left turn <b>do</b>       <math>H.\text{POPBACK}()</math>     <b>end while</b>     <math>H.\text{APPEND}(v)</math>   <b>end for</b>   <math>H.\text{POPBACK}()</math>   <b>return</b> <math>H</math> <b>end procedure</b> </pre>	<p>▷ Returns the partial convex hull left to <math>\overrightarrow{pq}</math>, including <math>p</math> but excluding <math>q</math>.</p> <p>▷ Take only points left to <math>\overrightarrow{pq}</math></p> <p>▷ Remove last element from <math>H</math></p> <p>▷ <math>q</math> is last element in <math>H</math>, remove it</p>

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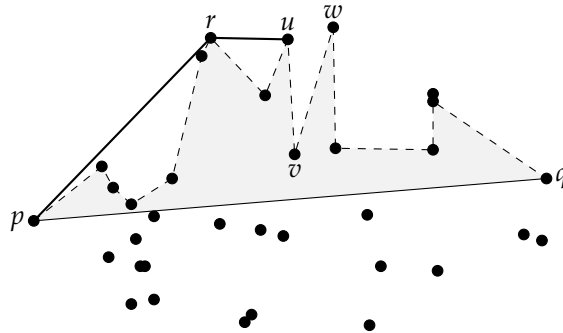


Figure 6.5: The Graham scan algorithm makes sure that while computing the upper part of the convex hull we only make right turns.



so-called Delaunay triangulations<sup>7</sup>, which again have particularly nice properties for finite element methods, which again are used to solve differential equations, which again are used for numerical simulation of all kind of physical systems.

As another example, suppose we are given a point set  $S$  and a convex polygon  $P$ . We would like to test whether  $S$  fits into  $P$ . The answer is “yes” if and only if  $\text{conv } S$  fits into  $P$ . Hence, we can compute the convex hull of  $S$  first and only make the check for the vertices of the convex hull. If we do many such tests for different  $P$  then the preprocessing step of computing  $\text{conv } S$  is done only once and can be reused for every new polygon  $P$ .

There are two general ideas to learn from the above example: (i) The convex hull can sometimes be used to speed up certain operations and (ii) typically problems are much easier to solve if the input is in some sense “convex”. For instance, testing whether a point is in a convex polygon is much simpler than testing whether a point is inside a non-convex polygon. Computing a triangulation of a convex polygon is much simpler than computing a triangulation of a non-convex polygon. Motion planning for a convex robot is much simpler than for a non-convex robot.

So assume we want to test whether two complex three-dimensional objects intersect, e.g., for collision detection in a 3D racing game. Further assume that most of the time the answer is “no”. We can speed up the complex task by first testing whether the convex hulls of the complex objects intersect, which is faster and simpler. Only if the answer is “yes” – we assume this happens infrequently – we have to make the slower and more complex test for the original objects.

Software packages like `scipy` for Python or `MATLAB` provide convex hull implementations. The following lines are from a Python interpreter shell. The `ConvexHull()` implementation is based on the `qhull` [2] library:

```
>>> import numpy as np
>>> from scipy.spatial import ConvexHull
>>> points = np.array([[0, 0], [1, 0], [1, 1], [0, 1], [0.5, 0.5]])
>>> hull = ConvexHull(points)
>>> points[hull.vertices]
array([[0., 0.],
       [1., 0.],
       [1., 1.],
       [0., 1.]])
```

---

<sup>7</sup>One can vertically lift the input points in the plane on a paraboloid one dimension higher, compute the convex hull there, and project the edges back onto the plane, which gives the Delaunay triangulation. This works for points in  $\mathbb{R}^d$  lifted to a paraboloid in  $\mathbb{R}^{d+1}$ . See also section 9.2.2.



# Range searching

## 7.1 Introduction

Consider the following task: We are given a large number  $n$  of points in the plane  $\mathbb{R}^2$  and we would like to cleanup the dataset by removing duplicate points. A simple algorithm could iteratively construct a clean set  $C$  of points by starting with the empty set  $\emptyset$  and iteratively adding a new point  $q$  to  $C$  if the closest point  $p \in C$  is farther away than an  $\varepsilon > 0$ . Denoting by  $d(p, q)$  the Euclidean distance between  $p$  and  $q$ , we have the following algorithm:

```

 $C \leftarrow \emptyset$ 
for  $q \in P$  do
  if  $C = \emptyset \vee \min_{p \in C} d(p, q) \geq \varepsilon$  then
    INSERT( $C, q$ )

```

A core operation in the above algorithm is to compute  $\min_{p \in C} d(p, q)$ . We call this a *nearest neighbor search* for a query point  $q$ . If we do it the naive way it takes time linear in the size of  $C$ , which makes the clean up algorithm quadratic time. But we can do much better!

We introduce data structures that can process  $C$  in order to allow so-called *range searching*: Given a query region  $Q$  the data structure returns all points of  $C$  contained in  $Q$ . Often  $Q$  is an axis-aligned rectangle, in which case we speak of *orthogonal range searching*. For our cleanup algorithm, we now set  $Q$  to a square of side length  $2\varepsilon$  and center  $q$  and instead compute  $\min_{p \in Q} d(p, q)$ . Assuming that  $Q$  contains a constant number of points of  $C$  only, the cleanup algorithm runs in linear time now.

## 7.2 Geometric hashing

A simple but in practice often efficient method is geometric hashing. The name is taken from *hash tables* and the idea is similar: Instead of considering the full problem, we “hash” the input data into buckets of smaller size, which allows us to consider the problem only in a single (or few) buckets. We describe the technique in two dimensions, but it is obvious how to extend it to higher dimension.

**The data structure.** So assume that we have a point set  $C$  of size  $n$  that fits into some axis-aligned rectangular region  $R$ . We now partition  $R$  into cells by a regular  $k \times m$  grid, see fig. 7.1 So each cell covers a subregion of  $R$  and for each cell we maintain a list of objects, namely points of  $C$ . That is, each point  $p \in C$  is registered at the cell in which it resides.

**Range searching.** A range query for a rectangular range  $Q$  now works as follows: Determine all cells of the geometric hash that intersect with  $Q$  and report every point in those cells that is actually contained in  $Q$ .

**Analysis.** The geometric hash is of an advantage if only a significantly smaller fraction of the set  $C$  of points needs to be considered. Whether this is the case depends (i) on the distribution of the point set  $C$  and (ii) on our choice of  $m$  and  $k$ .

In a lucky situation the point set  $C$  is distributed uniformly over  $R$ . Assume further that we choose  $m$  and  $k$  such that the cells are close to a square and  $m \cdot k$  is linear. Hence, on average a cell contains a constant number  $n/m \cdot k$  of points and if  $Q$  is small such that it covers only a constant number of cells then we can answer the range query in constant time. More generally, the runtime is linear in the size of  $Q$ , i.e., in the number of cells intersected by  $Q$ .

We do not make  $m \cdot k$  super-linear as we would pay super-linear space and time, even though they are mostly empty. If  $m \cdot k$  is sub-linear then we still have linear space complexity, simply to store all points. However, each cell now contains super-constant many points and hence it takes super-constant time per cell for a range query.

If the point set is not “nicely” distributed, such that the points concentrate on some cells, we lose the advantage of geometric hashing. In particular, if some cells contain a linear number of points then we are essentially as good as the naive solution in terms of time complexity when we consider those cells. Fortunately, in many data sets of real-world applications points are quite nicely distributed.

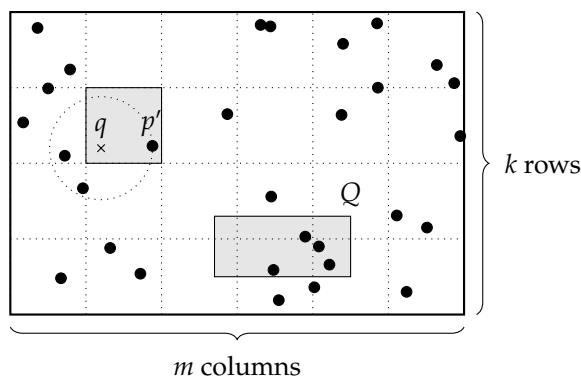


Figure 7.1: Geometric hashing for a point set in a rectangular region. It can be used for range queries for a query range  $Q$  or for nearest neighbor searches for a query point  $q$ . There is a candidate point  $p'$  in the cell of the query point  $q$  but the closest point is different to  $p'$ .

**Nearest neighbor search.** For a query point  $q \in R$  we would like to find the closest point  $p \in C$ . First, we find a candidate point  $p'$  for being the closest point in  $C$ : We determine the cell of the query point  $q$ , see the shaded area in fig. 7.1. If this cell contains at least one point then we determine the point  $p'$  closest to  $q$  within this cell. If the cell was empty, we consider the ring of neighboring cells for a candidate point. If these are also empty, we successively increase the search radius by adding another ring of cells. At some point we find a candidate  $p'$  that is the closest point within the considered cells, unless the entire geometric hash is empty.

Note that  $p'$  is not necessarily the closest point to  $q$  of all points in  $C$ , as fig. 7.1 illustrates. Hence we consider all cells that are intersected by the disk passing  $p'$  and centered at  $q$ . Within

these cells we find the point closest to  $q$  among all points in  $C$ .

**Bounded point query.** Some applications, like the initial data cleanup example, are actually a mix of a nearest neighbor search and a range query in the sense that we are interested in the nearest neighbor within a (possibly small) query range  $Q$ . When  $Q$  is small we can restrict our nearest neighbor search to those cells and do not need to increase search range if no point has been found.

## 7.3 Hierarchical data structures

When the point set  $C$  is far from being uniformly distributed, the geometric hash suffers from the fact that grid cells still cover the region  $R$  in a uniform fashion. So some cells may take many points while many cells may remain even empty. The advantage of geometric hashing is mitigated when cells contain super-constant many points and entirely erased when cells contain a linear number of points.

Hence, we seek for a decomposition scheme that is adaptive. Various hierarchical data structures can do so by refining some tessellation scheme as we go deeper in the hierarchy.

### 7.3.1 Quadrees

A quadtree is a tree where a node has either zero or four children. Each node  $N$  covers a rectangular region  $R(N)$ , with the root node covering the original region  $R$ . If a node  $N$  has children then  $R(N)$  is split into four quadrants at a split point in the middle of  $R(N)$  and each child node belongs to one of the four sub-rectangles, see fig. 7.2. The point set  $C$  is stored in the leaf nodes  $N$  of the quadtree, i.e.,  $N$  stores the points contained in  $R(N)$ . When a certain region contains more points than other regions then we increase the depth of the hierarchy further and make therefore the subdivision finer. In this sense, a quad tree is like geometric hashing with a locally adaptive resolution.

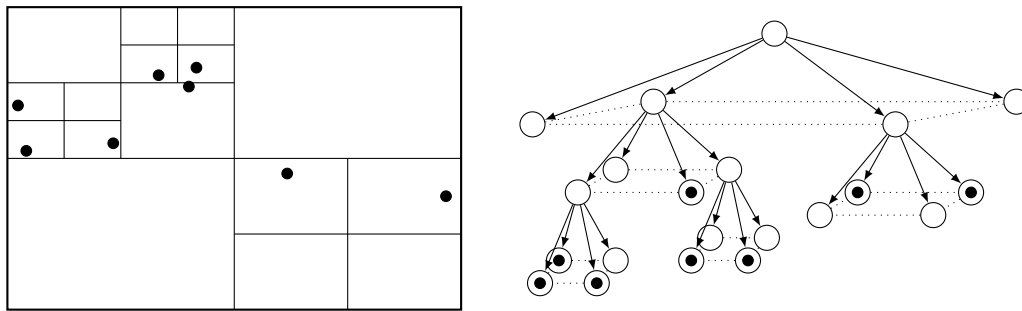


Figure 7.2: A quadtree with bucket capacity 1. Left: the cell decomposition of the quadtree. Right: The hierarchy of nodes, where each node covers a rectangular cell. The leaf nodes that contain a point are marked.

When we insert a new point  $p$  to the quadtree we traverse the quadtree from the root node down the hierarchy until we reached the leaf node  $N$  with  $p \in R(N)$  and we add  $p$  to the node  $N$ . The question arises when to subdivide a leaf node. Similar to B-trees each (leaf) node has a fixed bucket capacity. If a new point  $p$  is to be added to the leaf node  $N$  that has reached its capacity then  $N$  is subdivided – we add four children – and  $p$  is instead inserted into the corresponding

child node  $N'$  of  $N$ . It may happen that all points of  $N$  are actually located in  $R(N') \subseteq R(N)$ , so now  $N'$  has to be subdivided, and so forth. In fig. 7.2 we used a bucket size of 1, but in practice we would choose it larger.

When we perform a range query for an axis-aligned rectangular query range  $Q$ , we recursively traverse the quadtree top down starting at the root node. When we visit a node  $N$  and  $R(N)$  intersects  $Q$  we have two cases: If  $N$  is a leaf node then we report all points of  $N$  that are contained in  $Q$ . If  $N$  is no leaf node then we recursively repeat for every child  $N'$  of  $N$  for which  $R(N')$  intersects  $Q$ .

We can generalize a quadtree directly to  $\mathbb{R}^3$ , but now a node has eight children: One child for each octant at a split point. The resulting data structure is called an *octree*.

### 7.3.2 k-d trees

If we would not operate on the plane but on the one dimensional space  $\mathbb{R}$  then we could use ordinary binary trees for range searching. For points in  $\mathbb{R}^d$  with  $d \geq 2$  we can use ordinary binary trees only if we choose one particular spatial direction to define a sorting order of the points, but in general this does not help for orthogonal range searching.

A k-d tree organizes the points of  $C$  as a binary tree, but we switch the sorting direction level-wise between the coordinate axes. In fig. 7.3 we illustrate an example for  $\mathbb{R}^2$ . The root node  $a$  is in the first level, so it divides the point set into left and right: All points in the first subtree of  $a$  are geometrically left to  $a$ , which are  $b, d, e, h$ . All points in the second subtree are geometrically right to  $a$ . The node  $b$  is in the second level, so it divides the remaining point set into below and above: All points in the first (second) subtree of  $b$  are below (above)  $b$ . Similar for node  $c$ . The node  $d$  is in the third level, so it divides into left and right again: The node  $h$  is in the right subtree of  $d$  because it is geometrically right of  $d$ .

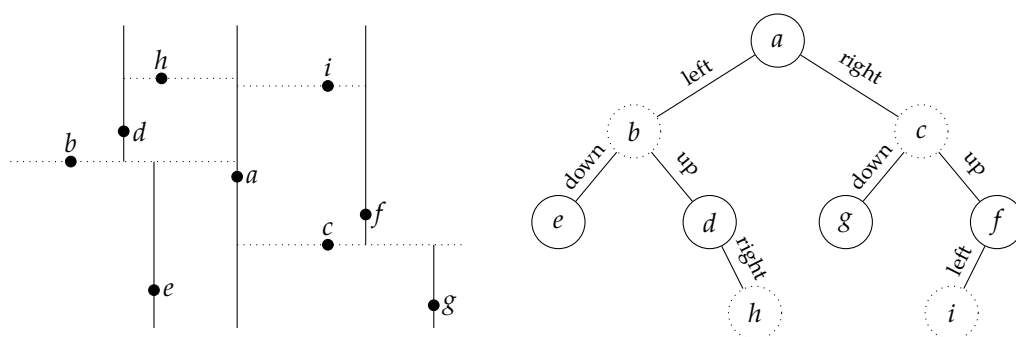


Figure 7.3: A k-d tree for a point set in  $\mathbb{R}^2$ . Left: The geometric tessellation scheme of the k-d tree. Right: The node hierarchy where every other level corresponds to a split along a different coordinate axis. Dashed lines on the left belong to dashed nodes on the right.

An orthogonal range search for a range  $Q$  is done by traversing the tree. In fig. 7.3 this means the following: If  $a$  is in  $Q$  then we report  $a$ . If  $Q$  reaches to the left (or right) of  $a$  then we recursively repeat for the left (or right) subtree of  $a$ . At the next level we do the same, only left/right is replaced by below/above.

The range search is fast if we can drop large subtrees in the traversal of the k-d tree. For this reason we are interested in balanced k-d trees. If we compute a k-d tree from scratch we therefore start by sorting the point set by  $x$ -coordinates and choose the median point as root. We

then take the left (right, resp.) subset, sort by  $y$ -coordinate, and again take the median as root of the subtree, and so on.

Recall that for quadtrees we have an initial region  $R$  in which the points lie, but  $k$ -d trees do not need such a thing. Also the location of the splitting is given by  $R$  for quadtrees, whereas for  $k$ -d trees the splitting lines are determined by the points of the point set.





# Graphs

Graphs consist of vertices and edges between the vertices. They are a fundamental concept in computer science. All kind of objects can be depicted as graphs, like networks, relations, dependencies, geometric objects, programs, neural nets and so on. Graph theory is a large discipline. We will only introduce a small fraction here.

## 8.1 Basic notions

A *graph* consists of a finite set  $V$  of vertices and a finite set  $E$  of edges, where an edge is a connection between two vertices  $u, v \in V$ . We distinguish between *undirected graphs* and *directed graphs*, depending on whether the edges have a direction or not. A directed graph is often also called *digraph*. Undirected graphs have undirected edges  $\{u, v\}$ . Note that  $\{u, v\} = \{v, u\}$  as orders of elements in sets are irrelevant. Directed graphs have directed edges  $(u, v)$ . Note that  $(u, v) \neq (v, u)$  when  $u \neq v$ , because pairs (as 2-tuples) are ordered. More formally, we can define graphs as follows:

**Definition 3.** An (undirected) graph  $G$  is a pair  $(V, E)$  of a finite vertex set  $V$  and a finite edge set  $E \subseteq \{\{u, v\} : u, v \in V\}$ . A directed graph  $G$  is a pair  $(V, E)$  with a finite vertex set  $V$  and a finite edge set  $E \subseteq \{(u, v) : u, v \in V\}$ .

From now on, if we just say graph, we mean undirected graph, unless we made it clear that we mean both. Some graphs are very special and we give them names. For instance, the *complete graph*  $K_n$  is a graph with  $n$  vertices and all possible edges, which are  $\frac{n(n-1)}{2}$  many. Other special graphs are regular graphs, bipartite graphs, Petersen graph, star graphs, wheel graphs, and many more.



Figure 8.1: An undirected graph and a directed graph on the vertex set  $V = \{0, 1, 2, 3, 4, 5\}$ .

Graphs are typically illustrated by diagrams as in fig. 8.1, where directed edges are illustrated by arrows and undirected edges by lines. We call this the *drawing* of a graph. Note that the

position of the vertices or geometry of the lines play no role for the graph; these are only details of one possible drawing. For the graph per se, we are purely interested in the combinatorial structure of the graph, i.e., whether vertices are connected to each other. In fig. 8.5a we see two different drawings of the complete graph  $K_4$ .

A *loop* is an edge from a vertex to itself. Often loops are excluded by definition and we speak of a *simple* graph to stress this point. If we take a digraph and forget about the edge directions then we obtain the *underlying (undirected) graph*. The underlying graph of the digraph in fig. 8.1b is the one in fig. 8.1a. (Note that the two directed edges  $(1, 2)$  and  $(2, 1)$  become the same undirected edge  $\{1, 2\}$ .)

We say that an edge between  $u$  and  $v$  is *incident* to  $u$  and  $v$ . Vice versa, vertices are *adjacent* if there is an edge between them. For an undirected graph we call the number of edges incident to a vertex  $u$  the degree  $d(u)$  of  $u$ . (For non-simple graphs, a loop is counted twice for the degree.) A vertex  $v$  of degree  $d(v) = 0$  is called *isolated*. In fig. 8.1a the vertex 0 is isolated and the vertex 3 has degree 4. We call a graph with every vertex of degree  $r$  a  *$r$ -regular graph*. The complete graph  $K_n$  is a  $(n - 1)$ -regular graph.

The vertex degrees and the number of edges of undirected graphs are in a relationship: When we insert an edge between  $u$  and  $v$  then the degree of  $u$  and  $v$  has been incremented. That leads to the following lemma, also known as the *degree formula*:

**Lemma 1.** *For an undirected graph  $(V, E)$  it holds that  $\sum_{v \in V} d(v) = 2|E|$ .*

In fig. 8.1a the sum is 10. There is also a nice counting argument for this lemma: Consider placing a dot at each “end” of the edge. How many dots did we place? From one point of view, we place  $2|E|$  dots because two dots per edge. On the other hand, at each vertex  $v$  we placed  $d(v)$  dots, so  $\sum_{v \in V} d(v)$  dots in total. Will use a similar argument later for triangulations in section 8.4.2.

From lemma 1 we also see that if we remove from  $\sum_{v \in V} d(v)$  all vertices of even degree, then the sum is still even. What remains is an even sum of odd degrees. So the number of summands must be even. This is called the *handshaking lemma*:

**Lemma 2** (Handshaking lemma). *The number of odd-degrees vertices in an undirected graph is even.*

The handshaking lemma says that at a party the number of people, shaking hands an odd number of times, is even. This example also shows a typical way how graphs are used as a modeling language: There are objects that are in relation to each other and we model this as a graph with the objects being the vertices and the relation being an edge. If the relation has a “direction” then we have a digraph, like for dependencies of tasks in a project.

For directed graphs, the *indegree*  $d^+(v)$  of a vertex  $v$  is the number of edges  $(\cdot, v)$  pointing to  $v$  and the *outdegree*  $d^-(v)$  of a vertex  $v$  is the number of edges  $(v, \cdot)$  pointing away from  $v$ . A vertex  $v$ , where indegree and outdegree are both zero, is called *isolated* again. In fig. 8.1b the vertex 0 is isolated and  $d^+(1) = 2$  and  $d^-(1) = 1$ .

## 8.2 Paths, cycles and trees

Many algorithms and problems consider different ways to traverse a graph, i.e., to move from vertex to vertex in specific ways. This is relevant for shortest paths or for depth-first or breadth-first searches and so on. The following definitions introduce different types of “wandering” around:

**Definition 4.** Let  $G = (V, E)$  denote a undirected or directed graph. A *walk*<sup>1</sup> from  $v_0 \in V$  to  $v_n \in V$  is a vertex sequence  $(v_0, \dots, v_n)$  such that for all  $0 \leq i < n$  the edge from  $v_i$  to  $v_{i+1}$  is an edge in  $E$ . A *tour*<sup>2</sup> is a walk with all edges being pairwise distinct. A *path*<sup>3</sup> is a walk with all vertices being pairwise distinct, except maybe  $v_0$  and  $v_n$ . We call  $n$  the length of the walk, tour or path, respectively. A *closed walk*, *tour* or *path* goes from a vertex  $v_0$  to the same vertex  $v_n = v_0$ .

The above definition works for directed and undirected graphs. In the following we will discuss undirected graphs only. Remember that a tour does not visit an edge twice, just like a good motorcycle tour. And a path does not visit a place (vertex) twice, in the sense it does not cross itself. See fig. 8.2 for examples.

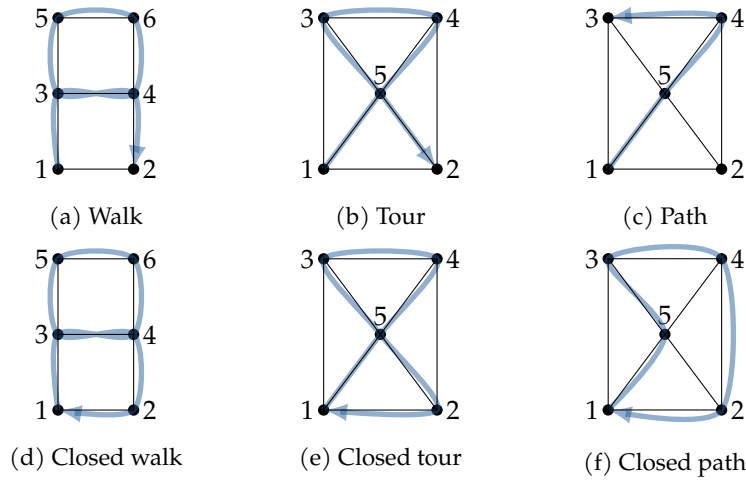


Figure 8.2: Closed and not closed walks, tours and paths.

By means of a walk we can define what we mean when a graph is connected. That is, we can go from any vertex to any other vertex by a walk. Actually, if there is a walk from a vertex  $u$  to a vertex  $v$  then there is also a path. Whenever the walk crosses itself at a vertex  $w$  then we can cut off the detour from  $w$  to  $w$  and obtain a shorter walk, until there are not any crossings anymore. That is, we transform a walk  $(u, \dots, w, \dots, w, \dots, v)$  into a walk  $(u, \dots, w, \dots, v)$  where  $w$  does not occur multiple times. This leads to the following definition based on paths:

**Definition 5.** We call a graph  $(V, E)$  *connected* if for all pair of vertices  $u, v \in V$  there is a path from  $u$  to  $v$ .

The graph in fig. 8.1a is not connected; for instance there is no path between vertex 0 and vertex 1. However, if we would remove vertex 0 then the remaining graph is connected. Sometimes we need to refer to parts of a graph, which we call subgraph. Formally, a graph  $G' = (V', E')$  is called a *subgraph* of a graph  $G = (V, E)$  if  $V' \subseteq V$  and  $E' \subseteq E$ . A cycle is a special subgraph of a graph, i.e., it is the subgraph “traced out” by a closed path:

**Definition 6.** A *cycle* of an undirected graph  $(V, E)$  is a subgraph  $(V', E')$  with a vertex set  $V' = \{v_1, \dots, v_n\}$  of  $n$  vertices such that  $E' = \{\{v_1, v_2\}, \{v_2, v_3\}, \dots, \{v_{n-1}, v_n\}, \{v_n, v_1\}\}$ . We call  $n$  the *length* of the cycle.

<sup>1</sup>Dt. Wanderung

<sup>2</sup>Dt. Weg

<sup>3</sup>Dt. Pfad

Note that a cycle is very similar to but not the same as a closed path: A closed path has a definite start, but a cycle – as defined as a subgraph – has no such thing as a start. The graph in fig. 8.1a has only one cycle  $(V', E')$  with  $V' = \{1, 2, 3\}$  and  $E' = \{\{1, 2\}, \{2, 3\}, \{3, 1\}\}$ . But this graph has three closed paths, all tracing out the same cycle. Also note that we could have defined a cycle as a connected subgraph where every vertex has degree 2.

If the cycle happens to contain all vertices of the graph then we call it a *Hamiltonian cycle*. Testing whether a graph has a Hamiltonian cycle is one of the classical NP-complete problems,<sup>4</sup> so there is most likely no polynomial algorithm.

If a graph contains no cycle then we call the graph *acyclic* or a *forest*. A forest in general consists of multiple trees, or from a formal point of view, a tree is a connected forest:

**Definition 7.** A *tree* is a connected, acyclic graph. We call vertices of degree 1 the *leafs* or leaf vertices.

A tree has the property that between any two vertices there is exactly one path: There must be at least one because it is connected, but there cannot be two. If there would be two then at some vertex these paths would diverge and rejoin later, and this would form a cycle. In a tree the number of edges is also given by the number of vertices:

**Lemma 3.** For a tree  $(V, E)$  holds  $|E| = |V| - 1$ .

A first simple proof is based on induction following this idea: We construct the tree iteratively by a sequence of trees  $T_1, \dots, T_n$ , where  $T_k$  has  $k$  vertices. We start with  $T_1$  having 1 vertex and 0 edges, where the property holds. In each step we let the tree  $T_k$  grow to  $T_{k+1}$  by adding one more vertex and an edge, each time keeping the property  $|E| = |V| - 1$  invariant.

Another proof is based on *rooted trees*, where we turn the tree into a directed graph by choosing one vertex as the *root* and then orienting all edges in a way that the point away from the root. So in this rooted tree there is a single path from the root to any vertex; the paths lead way from the root.<sup>5</sup> Observe that every vertex has in-degree 1, except the root.<sup>6</sup> So we have as many non-root vertex as edges, and hence  $|E| = |V| - 1$ .

We can actually turn every connected graph  $G$  into a tree by cleverly removing edges without destroying connectedness but achieving acyclicity: As long as there still exists a cycle we remove an arbitrary edge of the cycle, and repeat. Removing an edge of a cycle cannot destroy connectedness. What remains is a tree that “spans” the original  $G$ , which we call *spanning tree*:

**Definition 8.** We call a subgraph  $G' = (V', E')$  of a graph  $(V, E)$  a *spanning subgraph* if  $G'$  is connected and  $V' = V$ . A *spanning tree* of a graph is a spanning subgraph that is a tree.

Following this notation, we could have defined a Hamiltonian cycle as a spanning cycle. By definition, only connected graphs can have a spanning subgraph, let alone a spanning tree or a Hamiltonian cycle. Observe that a spanning tree  $T$  of a graph  $G = (V, E)$  cannot have more edges than  $G$ . The following corollary must therefore hold, otherwise  $T$  cannot fulfill lemma 3:

**Corollary 1.** Connected graphs  $(V, E)$  fulfill  $|E| \geq |V| - 1$ .

Spanning trees have numerous applications. One application is with communication networks and routing of packets, e.g., for the IP protocol. The communication nodes are linked

<sup>4</sup>In 1972, Richard Karp has proven for a variety of 21 computational decision problems that they are in the complexity class NP-complete. Unless the complexity class P would equal NP, there is polynomial time algorithm for any NP-hard problem, which includes the NP-complete problems. In fact, any NP-hard problem can be reduced to every NP-complete problem.

<sup>5</sup>All roads lead to Rome, but for rooted trees it is the other way round.

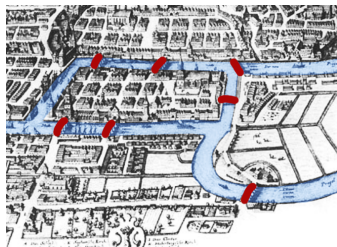
<sup>6</sup>And the leafs have out-degree 0.

together in a meshing network. To avoid routing loops, many protocols compute a spanning tree, most notably the Spanning Tree Protocol and variants of it. Many applications of spanning trees are actually using minimum spanning trees for weighted graphs, see section 8.3.

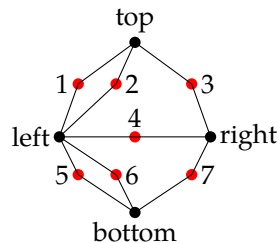
The discipline of graph theory surfaced through Leonhard Euler investigating the problem of the seven bridges of Königsberg, see fig. 8.3a. He was asked to find a route through Königsberg that would visit each bridge only once.<sup>7</sup> In the modern language of graph theory, we ask for a so-called Eulerian tour:

**Definition 9.** An *Eulerian tour* of a graph is a tour that visits all edges.<sup>8</sup>

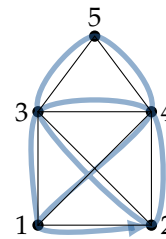
In fig. 8.3b we model the situation as a graph with every island and bridge being a vertex. Is there an Eulerian tour for this graph? The answer is “no”. But how can we prove? An algorithmic approach would be to come up with an algorithm to exhaustively search for Eulerian tours and find that the algorithm would yield no solution. A better approach is to learn something about the problem structure itself.



(a) Seven bridges of Königsberg. Based on image by Merian-Erben, public domain



(b) Graph of Königsberg



(c) A house in one stroke

Figure 8.3: The Königsberg bridge problem and Eulerian tours of graphs.

Say there would be an Eulerian tour  $(v_0, \dots, v_n)$  for a graph  $G$ . Then we observe that each vertex  $v_1, \dots, v_{n-1}$  is entered by one edge and exited by another. It may also be revisited later again, but for each visit we need two different edges. That means that the degree must be even. Only the degree of the first vertex  $v_1$  and the last vertex  $v_n$  must be odd when the Eulerian tour is not closed, and it must be even otherwise, i.e., when  $v_1 = v_n$ . This property is necessary. It is also sufficient, because we can essentially construct an Euler tour by traversing the graph arbitrarily along non-visited edges. Only for non-closed Eulerian tours we have to start at an odd-degree vertex. This gives us the following lemma:

**Lemma 4.** A connected graph has a closed Eulerian tour if and only if all vertices are of even degree and a non-closed Eulerian tour if and only if exactly two vertices are of odd degree.

In fig. 8.3b all vertices corresponding to islands have odd degree, so there is no Eulerian tour. Another commonly known riddle is shown in fig. 8.3c, where we shall draw this house figure in one stroke without tracing a line twice. That is, we again ask for an Eulerian tour, which exists: The vertices 1 and 2 are of odd degree, so we start at either one. The shown solution is the tour  $(1, 3, 4, 2, 3, 5, 4, 1, 2)$ , but we can find other solutions by starting at any odd-degree vertex and simply continuing with any unvisited edge until we reach the other odd-degree vertex.

<sup>7</sup>The Königsberg bridge problem also marks the start of topology, which is in some sense geometry without precise lengths and locations of objects. The length of a bridge is irrelevant for this problem.

<sup>8</sup>Eulerian tours are often also called Eulerian paths in literature.

Riddles like in fig. 8.3 can be considered to be part of so-called *recreational mathematics*. But Eulerian tours also have industrial applications, like assembling DNA fragments, CMOS circuit design and unfolding polyhedral surfaces [6], e.g., for CAD/CAM applications.

### 8.3 Weighted graphs

The edges of a graph put vertices into relation.<sup>9</sup> Often these relations carry some quantity, i.e., the time to travel between cities, the bandwidth between network nodes, or the probabilities between events in a *Bayesian network*. We call this quantity the *weight* and formalize it by a function  $w: E \rightarrow \mathbb{R}$  on the edge set  $E$ .

**Definition 10.** A *weighted graph*  $(G, w)$  is a pair of a graph  $G = (V, E)$  and a weight function  $w: E \rightarrow \mathbb{R}$ . Likewise we define a *weighted digraph*.

Sometimes we want to stress the point that we put weights on the edges and speak of an *edge-weighted graph*. A weighted digraph is also called *network*. It is also convenient to write  $w(u, v)$  instead of  $w((u, v))$  when there is an edge from  $u$  to  $v$ . What follows holds for undirected and directed graphs likewise. We draw weighted graphs by labeling the edges by their weight, like in fig. 8.4. Depending on the application a weight of zero is often equivalent to an edge being absent.

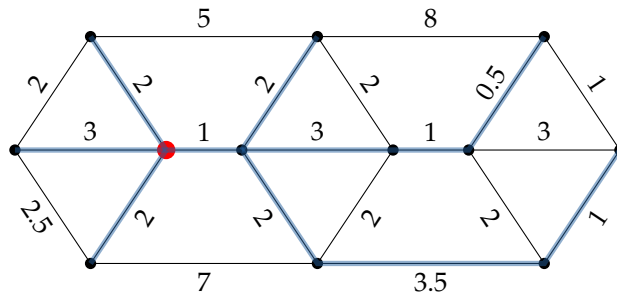


Figure 8.4: The rooted tree of shortest paths by Dijkstra. The source is marked red.

**Shortest paths.** We can now take different notions we know for undirected and directed graphs and ask for minimum-weight variants of it. Most prominently, we might be interested in a walk from a vertex  $u$  to a vertex  $v$  of minimum total weight. More formally, for a walk  $(v_0, \dots, v_n)$  we call  $\sum_{i=1}^n w(v_{i-1}, v_i)$  the *length* of the walk.

For most applications it makes sense to have the weights being non-negative. If weights can be negative then weight-minimizing instances, like walks, may not exist. For instance, if there is a cycle of negative total weight, then a weight-minimizing walk would keep spinning within this cycle indefinitely to add up negative lengths.

Let us assume weights are all positive. If there is walk between  $u$  and  $v$  then there is also a walk of minimum length. This minimum-length walk is actually a path: If the walk would revisit a vertex  $z$  then it cannot be of minimum length, because we could cut off the detour from  $z$  to

<sup>9</sup>There is actually a one-to-one correspondence between digraphs and relations. Formally, a relation  $R$  between a set  $A$  and a set  $B$  is a subset of the Cartesian product of  $A$  and  $B$ , i.e.,  $R \subseteq A \times B$ . Hence, for a digraph  $(V, E)$  on a vertex set  $V$ , we can see  $E \subseteq V \times V$  as a relation, and vice versa. Symmetric relations, i.e.,  $(a, b) \in R \Leftrightarrow (b, a) \in R$  for all  $(a, b) \in A \times B$ , correspond to undirected graphs.

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**Algorithm 5** Dijkstra's algorithm for one-source  $u$  all-destinations shortest paths.

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```

procedure DIJKSTRA(vertex set  $V$ , weights  $w$ , source vertex  $u$ )
  for  $v \in V$  do
     $dist[v] \leftarrow \infty$                                 ▷ Distance of  $v$  to current tree
     $prev[v] \leftarrow \text{Null}$                              ▷ Predecessor in rooted tree
  end for
   $dist[u] \leftarrow 0$                                     ▷ Distance to source  $u$ 
  for  $v \in V$  do                                       ▷ Initialize priority queue  $Q$ 
     $Q.insert(v, dist[v])$ 
  end for
  while  $Q$  not empty do
     $u \leftarrow Q.pop()$                                 ▷ Get vertex  $u$  closest to tree
    for neighbors  $v$  of  $u$  do                            ▷ Check for a shortcut to  $v$  via  $u$ 
      if  $v \in Q$  then                                    ▷ For unprocessed vertices  $v$ 
         $d \leftarrow dist[u] + w(u, v)$ 
        if  $d < dist[v]$  then                                ▷ There is a shortcut of distance  $d$ 
           $dist[v] \leftarrow d$ 
           $prev[v] \leftarrow u$ 
           $Q.update(v, dist[v])$ 
        end if
      end if
    end for
  end while
  return  $dist, prev$ 
end procedure

```

---

$z$  and reduce the length.<sup>10</sup> Hence, we call a minimum-length walk between  $u$  and  $v$  the *shortest path*.<sup>11</sup> Furthermore, we call largest shortest path between any pair of vertices the *diameter* of the graph.

Shortest paths have many applications, not the least for vehicle routing in street networks. A well-known algorithm for the computation of shortest paths is the *Dijkstra algorithm*. What Dijkstra's algorithm does is actually computing all shortest paths from one source to all destinations. Dijkstra does this in a way that gives rise to a rooted tree with the source vertex as root, see fig. 8.4. In fact, the algorithm computes this tree by iteratively adding a vertex to the tree that has minimum distance to the source vertex. We encode this tree by remembering for each vertex  $v$  its predecessor. The algorithm is given in pseudo code in algorithm 5. Depending on the data structure we use for the priority queue and for the graph, we obtain different time complexities of the algorithm, with the simplest versions being in  $O(|V|^2)$ . All we said about shortest paths works for undirected and directed graphs alike.

**Minimum spanning trees.** For undirected graphs, also spanning trees can be considered in a weight-minimizing fashion: Given a weighted graph  $(G, w)$ , the *weight* of a subgraph  $(V', E')$  of  $G$  is defined as its total weight  $\sum_{e \in E'} w(e)$ . Then we can define a *minimum spanning tree* (MST) of a weighted graph  $(G, w)$  as a spanning tree of  $G$  of minimum weight. There are many ap-

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<sup>10</sup>Note that we assumed positive weights, not just non-negative weights. If weights can be zero then there could be a cycle of zero total weight, and a shortest walk could revisit vertices.

<sup>11</sup>In literature, often what we call a "walk" is called a "path", so double check the definition of a path.

plications of minimum spanning trees, like hierarchical clustering, broadcasting in computer networks, image registration and segmentation and many more.

We can incrementally construct a minimum spanning tree by adding a vertex to the current tree that by an edge of minimum weight. This is called *Prim's algorithm*. This is similar to Dijkstra, but for Dijkstra we consider the minimum distance to the source vertex, not to *any* vertex of the current tree. On the other hand, *Kruskal's algorithm* considers each vertex of being a trivial tree, and then merges trees to form larger trees via minimum weight edges until only one tree remains.

**Traveling salesperson problem.** A famous problem in computer science is the *traveling salesperson problem* (TSP).<sup>12</sup> A salesperson wants to visit every vertex in a graph exactly once in a closed walk of minimum length. That is, TSP asks for the minimum-weight Hamiltonian cycle, which is again NP-hard.

## 8.4 Planar graphs and geometric graphs

The concrete drawing of a graph was irrelevant so far. That is, the positions of the vertices and the geometric shapes of the edges were irrelevant. In the following, we will subsequently add more structure concerning the drawing of graphs.

### 8.4.1 Planar graphs

If we can draw a graph in the plane in a way such that edges do not cross then we call this a *planar graph* and such drawing is called a *planar embedding* of the graph into the plane. The complete graphs  $K_n$  are planar for  $n \leq 4$  and are not planar for  $n \geq 5$ . In fig. 8.5a we see two planar embeddings of the complete graph  $K_4$ . Planar graphs and planar embeddings have many applications, e.g., for wire routing of a circuit in PCB layouting. Testing whether a graph is planar or not is difficult.

If we consider a *convex polyhedron*<sup>13</sup> then the vertices and edges of the polyhedron form a graph, the so-called *edge graph* of the convex polyhedron. In fig. 8.5b we illustrate the edge graphs of the tetrahedron and the cube. One can prove that edge graphs of convex polyhedra are planar.<sup>14</sup>

If we consider a planar embedding of a planar graph  $G$  then the plane is tessellated into *faces* formed by the edges, see also fig. 8.5. The main theorem on planar graphs is given by *Euler's formula*<sup>15</sup>:

**Theorem 1.** For any connected, planar graph with  $v$  vertices,  $e$  edges and  $f$  faces it holds that

$$v - e + f = 2. \quad (8.1)$$

Here we also count the unbounded, infinitely large face as a face. It is called the *outer face*. In fig. 8.5a the outer face is a triangle in both cases and in fig. 8.5b the outer face is a quadrilateral. As an example, the edge graph of a cube has 8 vertices, 12 edges and 6 faces and  $8 - 12 + 6 = 2$  and the edge graph of a tetrahedron has 4 vertices, 4 faces and 6 edges and  $4 - 6 + 4 = 2$ .

<sup>12</sup>It used to be called *traveling salesman problem*.

<sup>13</sup>A convex polyhedron is the convex hull of finitely many points in  $\mathbb{R}^3$ , and likewise for a  $d$ -dimensional convex polyhedron in  $\mathbb{R}^d$ .

<sup>14</sup>Actually, Steinitz' theorem says that a graph is the edge graph of a convex polyhedra if and only if it is 3-connected and planar. That is, Steinitz' theorem completely characterizes the edge graphs of convex polyhedra. A graph is  $k$ -connected when the removal of any  $k$  vertices keeps the graph connected.

<sup>15</sup>Dt. Euler's Polyedersatz.



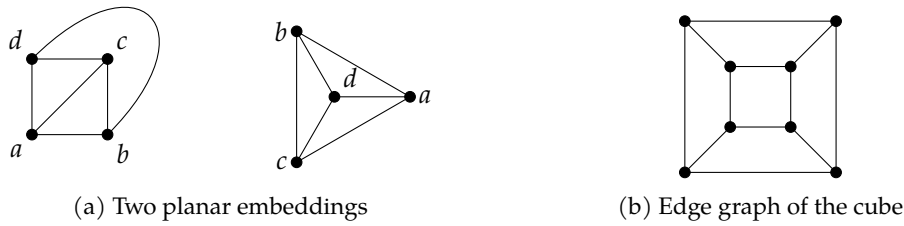


Figure 8.5: Planar graphs have a crossingfree drawing. Left: Two different embeddings of the same graph with four vertices  $a, b, c, d$ . It is the edge graph of the tetrahedron. Right: The edge graph of the cube with six quadrilateral faces.

In eq. (8.1) we see a certain symmetry concerning vertices and faces. Indeed, from a planar embedding of a graph  $G$ , we can form a *dual graph*  $G'$  by turning vertices in faces and vice versa: Each face  $f$  of  $G$  gives rise to a vertex  $v'$  of  $G'$  and if two faces  $f, g$  in  $G$  share an edge then we place an edge in  $G'$  between the vertices forming the duals of  $f$  and  $g$ . In this sense, we can think of “flipping” the edges of  $G$  to form the edges of  $G'$ . The dual of the dual of  $G$  is  $G$  again.<sup>16</sup> In fig. 8.6 we illustrated the dual graphs of fig. 8.5a. The dual of the cube graph is an octahedron graph. The dual of the tetrahedron graph is a tetrahedron graph; in this sense the tetrahedron is dual to itself.<sup>17</sup>

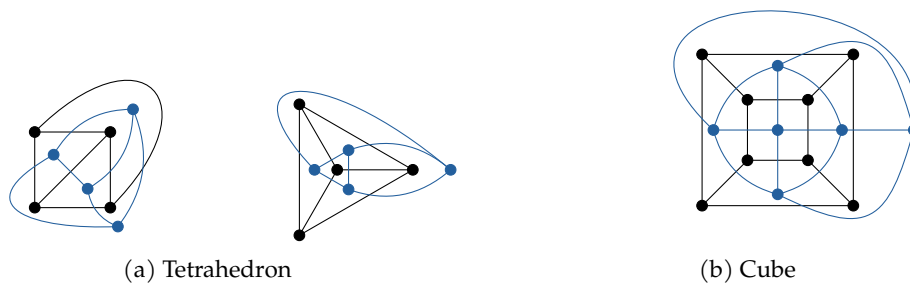


Figure 8.6: Dual graphs of (planar embeddings of) graphs in fig. 8.5a.

Dual graphs have many applications. One approach to compute unfoldings of polyhedral solids is to search for certain spanning trees of the dual of the edge graph. In fig. 9.4 we have the Delaunay triangulation as the dual of the Voronoi diagram, so we can easily compute the one from the other. But also for a mathematical analysis this duality is very useful. For instance, the regular structure of the Delaunay triangulation translates to regular properties of the Voronoi diagram (and vice versa) through duality.<sup>18</sup>

<sup>16</sup>This is an essential property of duality. For instance, we consider a point-line duality for the so-called Hough transform. Also here the dual of a dual is the original again.

<sup>17</sup>The dual of the icosahedron would be the dodecahedron. That is all five platonic solids have platonic solids as duals.

<sup>18</sup>Triangles in the Delaunay triangulation correspond to degree-3 vertices in the Voronoi diagram. By enforcing a triangle as outer face as well, we have a strong combinatorial property through lemma 5.

### 8.4.2 Geometric graphs

For planar graphs it matters that there is a planar drawing, a planar embedding, but the drawing itself is not of a main interest. We can add more geometry to graphs and also fix the way we draw the graph and speak of *geometric graphs*.

**Euclidean graph.** A natural way to pull in geometry to graphs is by embedding vertices into the plane and for each edge between a vertex  $u$  and vertex  $v$  we assign a weight equal to the Euclidean distance  $d(u, v)$  between the vertices. We call this a *Euclidean graph*. The *complete Euclidean graph* is then the complete, Euclidean graph of a vertex set given by a finite point set  $p_1, \dots, p_n \in \mathbb{R}^2$ .

The *Euclidean minimum spanning tree* (EMST) of a finite point set  $p_1, \dots, p_n \in \mathbb{R}^n$  is then the minimum spanning tree of the complete Euclidean graph. See fig. 8.8 for an example. Likewise the *Euclidean traveling salesperson problem* (ETSP) is then the traveling salesperson problem on the complete Euclidean graph. See fig. 8.7 for an example. We will revisit EMST and ETSP later in section 9.3.2 after we introduced Delaunay triangulations.

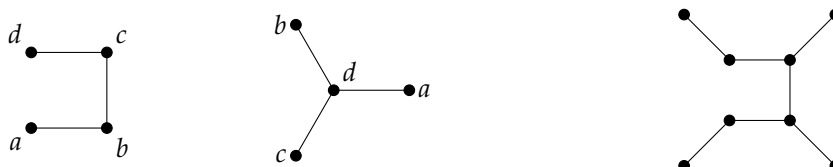


Figure 8.7: The Euclidean minimum spanning trees of the point sets in fig. 8.5.

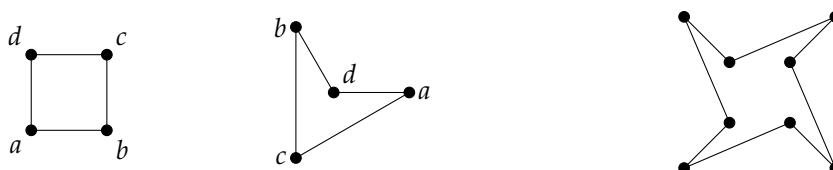


Figure 8.8: Solutions to the Euclidean TSP for the point sets in fig. 8.5.

**Planar straight-line graph.** Another prominent geometric graph is the *planar straight-line graph* (PSLG): We embed the vertices of the graph in the Euclidean plane, draw the edges as non-crossing straight-line segments. The PSLG as a weighted graph is a Euclidean graph, i.e., we assign the Euclidean lengths of the edges as weights. In fig. 8.5b we see a PSLG. As the weights are given by the Euclidean distance, the weights need not be explicitly displayed in a figure but are given implicitly.

A triangulation is a special PSLG. Given a set of points  $S \in \mathbb{R}^2$ , we define a *triangulation* of  $S$  as a maximal planar subdivision of the convex hull of  $S$ . Note that  $S$  may possess many triangulations.<sup>19</sup> The Delaunay triangulation is a special triangulation and will be introduced in section 9.1.2. See fig. 9.4 for an example.

<sup>19</sup>The number of triangulations is typically difficult to count. In the simple case of  $n + 2$  points in convex positions, there are  $C_n$  many triangulations, where  $C_n = \frac{1}{n+1} \binom{2n}{n}$  is the  $n$ -th Catalan number, which quickly becomes huge, i.e.,  $C_{10} = 16796$ ,  $C_{20} = 6564120420$ ,  $C_{30} = 3814986502092304$ .

All faces of a triangulation, except maybe the outer face, are triangles. Assume that also the outer face is a triangle. Then every edge belongs to two faces and every face has three edges. Draw a little dot on either side of an edge, then you have placed  $2e$  dots. On the other hand, each triangle received three dots, one from each edge, so we also placed  $3f$  dots and therefore  $2e = 3f$ . (We used a similar counting argument for the degree formula.) If we plug this into Euler's formula we get

$$6 = 3v - 3e + 3f = 3v - 3e + 2e = 3v - e$$

and therefore

$$e = 3v - 6.$$

Note that this only holds if all faces, including the outer face, form triangles, as in fig. 8.5a. However, since triangulating a non-triangular face only adds edges but no vertices, we obtain by eq. (8.1) for *any* planar graph the following:

**Lemma 5.** *For any connected, planar graph with  $v \geq 3$  vertices and  $e$  edges we have  $v - 1 \leq e \leq 3v - 6$ , with the first equality for a tree and the second equality if all faces are triangles.*

(Recall that  $e \geq v - 1$  is by corollary 1.) In particular, planar graphs possess at most a linear number of edges! Many algorithms for graphs have a time complexity that depends on the number of edges; they are faster on graphs with less edges. Hence, they perform better on planar graphs than arbitrary graphs. Prime examples are the computation of shortest paths<sup>20</sup> or minimum spanning trees<sup>21</sup>.

Based on the above inequality we can also bound the number of faces in a connected, planar graph, as  $f = e - v + 2 \leq 3v - 6 - v + 2 = 2v - 4$ .

**Corollary 2.** *For any connected, planar graph  $G$  with  $v \geq 3$  vertices and  $f$  faces we have  $1 \leq f \leq 2v - 4$ . Iff  $G$  is a tree we have  $f = 1$  and iff all faces of  $G$  are triangles we have  $f = 2v - 4$ .*

If  $G$  is a tree then there are no cycles and the only face is the outer face. If the connected, planar  $G$  is not a tree then  $G$  contains a cycle and then we have  $2 \leq f \leq 2v - 4$ . Then both equalities hold, i.e.,  $2 = f = 2v - 4$ , when  $G$  is a single triangle; then it is a cycle and all faces are triangles.

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<sup>20</sup>Take for instance Dijkstra's algorithm.

<sup>21</sup>Take for instance Kruskal's algorithm.



# Voronoi diagram and Delaunay triangulation

We would like to add a new power plant in a country to lower the load of the existing ones. To this end we would like to estimate the load of a power plant: We assume that households are uniformly distributed over the country and a household is served by its nearest power plant. So the load of a power plant is proportional to area of households where this plant is nearest to. What we receive is a geometric setup as illustrated in fig. 9.1, where the points are the power plants and the polygonal tessellation of the plane tells which households are served by which power plant. For instance, all households in the shaded, thick polygon are served by  $p$ .

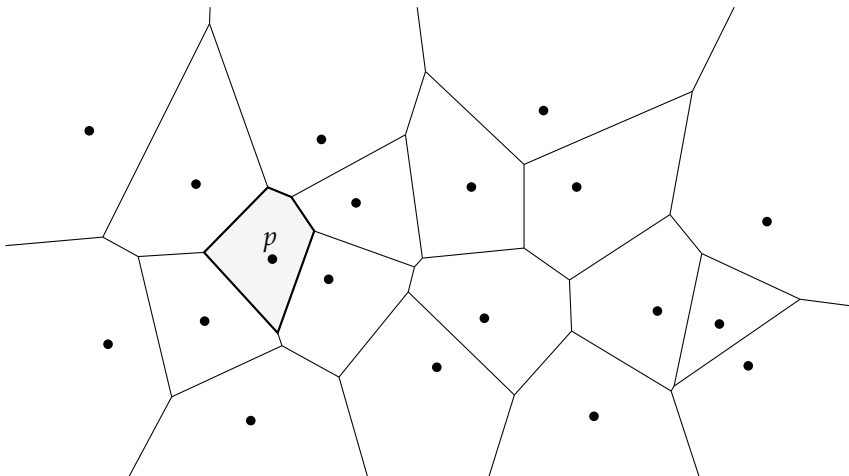


Figure 9.1: Voronoi diagram of points. The Voronoi region of  $p$  is shaded in gray and its boundary, the Voronoi polygon, is depicted thick.

## 9.1 Definition and properties

### 9.1.1 Voronoi diagram of points

A very similar problem formulation is known as the *post office problem*: The points in the plane, which are called *sites*, are post offices. A client posts a letter at its nearest post office, so for a post

office  $p$  its service region is the set of points where  $p$  is the nearest neighbor.

This leads us to the definition of a *Voronoi diagram* of a set  $S$  of point sites  $s_1, \dots, s_n$  in the Euclidean plane. For a site  $s \in S$  we define its *Voronoi region*  $VR(s)$  as the nearest-neighbor region of  $s$  among  $S$ :

$$VR(s) = \{p \in \mathbb{R}^2 : d(p, s) \leq d(p, s') \ \forall s' \in S\}. \quad (9.1)$$

If the notation is ambiguous on  $S$  then we add  $S$  as subindex and write  $VR_S(s)$ . For the Euclidean plane the distance  $d$  is given by

$$d(p, q) = \|p - q\| = \sqrt{(p_x - q_x)^2 + (p_y - q_y)^2}.$$

In an actual implementation we do not compute  $d(p, s) \leq d(p, s')$  but the equivalent comparison  $d(p, s)^2 \leq d(p, s')^2$  in order to get rid of the square root in the numerical computations, which is slow and inaccurate. We define the *Voronoi polygon*  $VP(s)$  as the boundary of  $VR(s)$ , which is denoted by  $VP(s) = \partial VR(s)$ .

**Definition 11.** The *Voronoi diagram*  $V(S)$  of a set  $S = \{s_1, \dots, s_n\}$  of sites in  $\mathbb{R}^2$  is defined as

$$V(S) = \bigcup_{s \in S} VP(s).$$

The Voronoi diagram has many very nice geometric properties. First we note that we can rephrase eq. (9.1) as

$$VR(s) = \bigcap_{\substack{s' \in S \\ s' \neq s}} H(s, s') \quad (9.2)$$

with

$$H(s, s') = \{p \in \mathbb{R}^2 : d(p, s) \leq d(p, s')\}.$$

The point set  $H(s, s')$  is a half plane with the bisector between  $s$  and  $s'$  as boundary, see fig. 9.2. Each point  $x$  on the bisector is equidistant to  $s$  and  $s'$ . From eq. (9.2) we learn that every Voronoi region is the intersection of half planes and therefore a convex polygon. However, some of them might be unbounded, i.e., infinitely large.

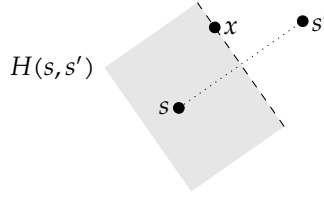


Figure 9.2: The half plane  $H(s, s')$  with the bisector between  $s$  and  $s'$  as boundary.

The Voronoi diagram  $V(S)$  tessellates the plane into convex polygonal cells<sup>1</sup>. We call the edges of  $V(S)$  the *Voronoi edges* and the vertices of  $V(S)$  the *Voronoi nodes*. In fig. 9.3a we illustrate a Voronoi node  $n$ , the incident Voronoi edges and the sites  $s_i$  of the incident Voronoi regions. Note that  $n$  lies on the Voronoi edge and bisector between  $s_1$  and  $s_2$ , so  $n$  is equidistant to both sites. But this also holds for all other Voronoi edges. Hence, a Voronoi node is equidistant to all sites of incident Voronoi regions.

<sup>1</sup>In some literature the Voronoi region is also called Voronoi cell.

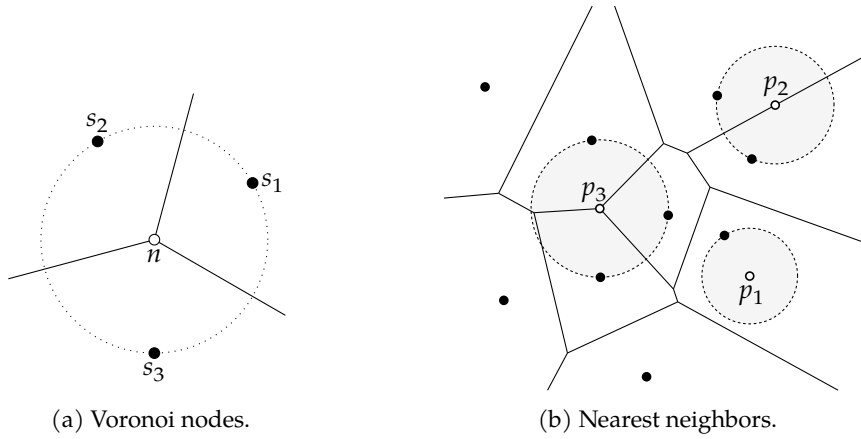


Figure 9.3: Left: A Voronoi node  $n$  has three or more incident Voronoi edges. All sites  $s_1, \dots, s_k$  of the incident Voronoi regions are equidistant to  $n$ . Right: The points  $p_1, p_2, p_3$  have one, two or more than two nearest neighbors in  $S$ .

Every point  $p$  in the plane has either one nearest neighbor  $s \in S$  or two nearest neighbors  $s_1, s_2 \in S$  or more than two. In the first case  $p$  lies in the interior of  $\text{VR}(s)$ , in second case  $p$  lies on a Voronoi edge and in the third case  $p$  lies on a Voronoi node, see fig. 9.3b.

### 9.1.2 Delaunay triangulation

We can also interpret  $V(S)$  as a planar graph, a PSLG in fact. Hence, we can consider the dual graph of  $V(S)$  as in fig. 9.4. What we obtain is the so-called *Delaunay triangulation*  $D(S)$  of the point set  $S$ . We call the line segments of the Delaunay triangulation the (*Delaunay*) edges.

Note that the Delaunay triangulation contains the convex hull of  $S$  as edges. Every Voronoi edge corresponds to a Delaunay edge. The infinitely long Voronoi edges are the Delaunay edges of the convex hull.

The Delaunay triangulation is a triangulation with particularly nice properties. If we consider the incident Voronoi edges to a Voronoi node  $n$  then each of them gives rise to a Delaunay edge. Hence, every Voronoi node gives rise to a Delaunay triangle, see fig. 9.5a.

In fact, if a Voronoi node is of higher degree than three – because more than four sites  $s_1, \dots, s_k$  are cocircular – then we do not obtain a triangle but a regular  $k$ -gon and we have to triangulate this  $k$ -gon (in an arbitrary way). Only in this case the Delaunay triangulation is not unique.

Another nice property is that the circumcircle of a Delaunay triangle does not contain any sites  $s$  in its interior. If this would be the case, the Voronoi node  $n$  to the Delaunay triangle would not have its defining sites as nearest neighbors but  $s$ , see fig. 9.5a. This property leads to a different definition of the Delaunay triangulation: For any three sites  $s_1, s_2, s_3$  whose circumcircle is empty we add a Delaunay triangle.<sup>2</sup>

In fig. 9.5b the left triangulation is not Delaunay for exactly this reason. However, we can perform an *edge flip* operation: We remove an edge, obtain a convex 4-gon, and re-triangulate this 4-gon the other way. If the resulting 4-gon would not be convex then re-triangulating it the other way would destroy planarity, so we can only do an edge flip if the resulting 4-gon is convex. It can be shown that a triangulation of  $n$  points can be turned into *any* other triangulation – in particular the Delaunay triangulation – using only  $O(n^2)$  edge flip operations.

<sup>2</sup>We have a special case if  $k \geq 4$  sites are cocircular. In such situations we have to triangulate the resulting  $k$ -gon.

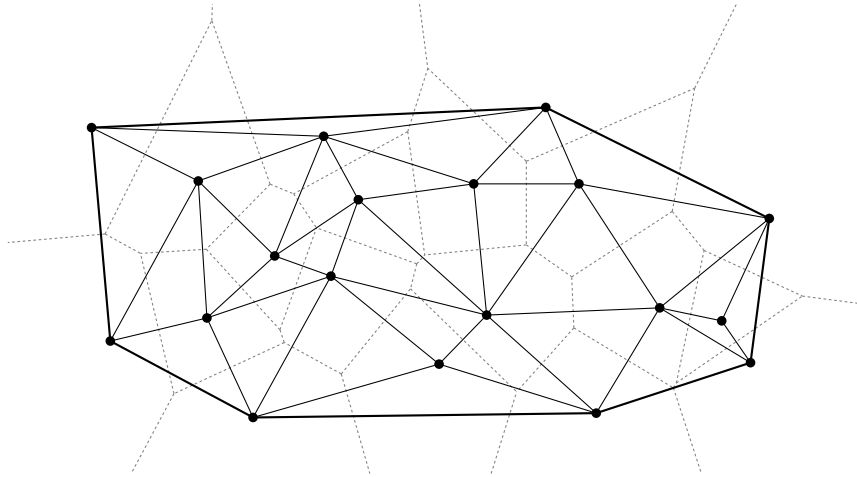


Figure 9.4: The Delaunay triangulation  $D(S)$  of a point set  $S$  is the dual graph of the Voronoi diagram  $V(S)$ .

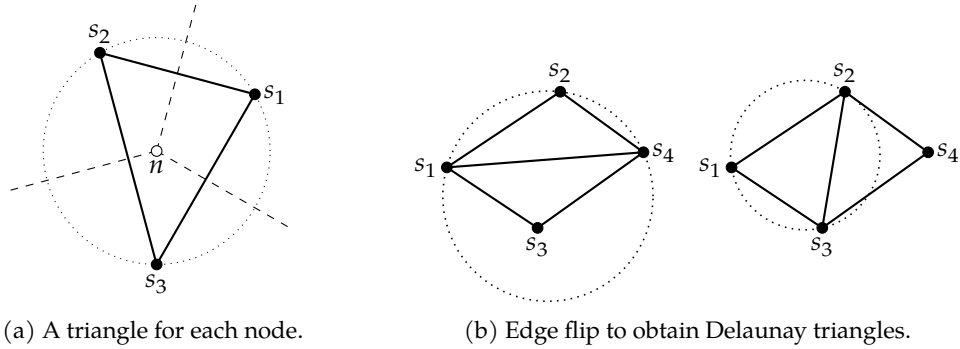


Figure 9.5: The circumcircles of Delaunay triangles are empty. Left: For every Voronoi node  $n$  there is a Delaunay triangle of the defining sites. Right: The triangle  $(s_1, s_2, s_4)$  is not Delaunay, but flipping the edge  $(s_1, s_4)$  creates Delaunay triangles.

The edge flip operation in fig. 9.5b makes the triangles more acute, closer to equilateral triangles. In fact, it can be shown that the Delaunay triangulation is optimal in the sense that among all triangulations the smallest angle over all its triangles is maximized. This makes the Delaunay triangle particularly “aesthetic” and, for instance, interesting for finite element methods.

## 9.2 Computation

### 9.2.1 Incremental construction of Voronoi diagrams

A simple algorithm to compute Voronoi diagrams is to construct it incrementally. If  $S$  contains at most three points, the Voronoi diagram is simple and looks like fig. 9.3a. If  $S$  contains more than three points, we can start with the first three, and iteratively add the remaining points.

So the problem we have to solve is the following: Given  $V(S)$  of a site set  $S$ , how to compute



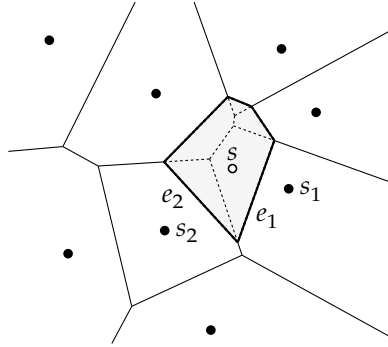


Figure 9.6: Inserting a site  $s$  creates a new Voronoi polygon  $VP(s)$  and removes the dashed line structure.

$V(S \cup \{s\})$  for a new site  $s \notin S$ ? Let us denote by  $S^+$  the new site set  $S \cup \{s\}$ . So how can we modify  $V(S)$  in order to obtain  $V(S^+)$ ? At the end  $V(S^+)$  has to contain a new Voronoi polygon  $VP_{S^+}(s)$ . The bisectors between the old sites remain unchanged, so many Voronoi edges will remain intact, some may be shortened, and some may be entirely deleted to clear space for  $VP_{S^+}(s)$ . In fig. 9.6 we illustrate this situation.

**Circular scan.** Let  $s_1 \in S$  be the<sup>3</sup> nearest neighbor of  $s$  among the old site set  $S$ . Since  $s \in VR_S(s_1)$ , some parts of the old Voronoi region  $VR_S(s_1)$  of  $s_1$  will be part of the new Voronoi region  $VR_{S^+}(s)$  of  $s$  and so the old region has to be truncated. More precisely, we consider the bisector between  $s_1$  and  $s$  and obtain an edge  $e_1$  of the new Voronoi polygon  $VP_{S^+}(s)$ . The edge  $e_1$  ends at an old Voronoi edge between  $s_1$  and a neighboring site  $s_2$ . The old Voronoi region  $VR_S(s_2)$  is therefore also truncated by the new Voronoi region of  $s$ , and we can again construct a Voronoi edge  $e_2$  on the bisector of  $s$  and  $s_2$ . We can keep doing that and eventually end up at  $s_1$  again, because we know that  $VP_{S^+}(s)$  is a convex polygon.

We call this traversal scheme of  $V(S)$  a *circular scan* around  $s$ . After we circularly constructed the new Voronoi polygon  $V_{S^+}(s)$  and removed the parts of the Voronoi edges enclosed by new polygon, we obtain the new Voronoi diagram  $V(S^+)$ .

**Topology-oriented construction.** The circular scan involves many geometric constructions that build upon each other: We compute a bisector line, intersect it with a Voronoi edge, construct a new point, and keep doing so in order to construct a whole sequence of new Voronoi edges  $e_1, e_2, \dots, e_k$ . In each step we *accumulate* numerical errors due to geometric computations, which are based on floating-point arithmetic.<sup>4</sup> Due to numerical inaccuracies the last edge  $e_k$  will not exactly meet with the first edge  $e_1$ . In fact, we may end up in a spiral of new Voronoi edges that actually fails to meet  $e_1$  again.

Sugihara [23] introduced a technique called *topology-oriented computation*. The general, abstract idea is to avoid geometric computations – and the continuous world as a whole – as far as possible and instead rely on discrete, integer-based information. In case of the incremental construction of Voronoi diagrams, we observe that the structure to be removed from  $V(S)$  is always

<sup>3</sup>In general, there could be many nearest neighbors if  $s$  sits on an edge or node of  $V(S)$ . In this case we take any such nearest neighbor and call it  $s_1$ .

<sup>4</sup>There are alternatives to floating-point arithmetic, like Exact Geometric Computation (EGC) based on libraries like Core or LEDA.

a tree, i.e., connected and free of cycles. Roughly speaking, if the dashed structure in fig. 9.6 would contain a cycle then a whole Voronoi polygon would be removed, which is impossible as every site has a Voronoi region.

We can exploit this fact for a topology-oriented insertion of a new site  $s$ : We again consider the site  $s_1$  whose Voronoi region  $VR_S(s_1)$  contains  $s$  and find a Voronoi node of  $VP_S(s_1)$  that is closer to  $s$  than  $s_1$ , which always exist. This node is definitely to be removed. Now we traverse  $V(S)$  and mark all nodes that are closer to  $s$  than their defining sites. Voronoi edges with both nodes marked are removed. Voronoi edges with only one marked node are truncated (partially removed). The key is now that if we would remove a whole cycle of Voronoi edges due to some numerical errors then we proactively avert that by breaking this cycle up at reasonable locations. That is, we *enforce* to remove a tree structure only. Therefore we help the implementation to produce topologically correct results; the implementation is *guided by* topological properties of Voronoi diagrams. Sugihara [23] demonstrated this technique for Voronoi diagrams, but the underlying idea is a powerful technique in general:

Avoid geometric and continuous computations, leverage topological and discrete information.

## 9.2.2 Complexity and implementations

Interpreting the Delaunay triangulation and the Voronoi diagram as a planar graph gives us some combinatorial properties that important regarding the computational complexity. First, by corollary 2, we know that there are only a linear number of Delaunay triangles. By duality, there are only a linear number of Voronoi nodes. And by lemma 5 there are only linear number of Voronoi edges (or Delaunay edges).

This insight is important for the time complexity of algorithms and space complexity to store Voronoi diagrams and Delaunay triangulations. In particular, it can be shown that if we construct  $V(S)$  incrementally and choose the points in a random fashion then the *expected* runtime is  $O(n \log n)$ . However, there are also deterministic  $O(n \log n)$  algorithms. Based on  $V(S)$  we can compute  $D(S)$  in  $O(n)$  time.

The qhull library – which is used by scipy and MATLAB – can actually compute  $V(S)$  and  $D(S)$  by means of the convex hull in higher dimensions. It can be shown that if we lift the point set  $S$  into  $\mathbb{R}^3$  by vertically lifting them on a paraboloid then their convex hull forms a polyhedron, whose edges projected back onto the plane gives the  $D(S)$ .

## 9.3 Applications

### 9.3.1 Terrain interpolation

Assume we are interested in some function  $f: D \rightarrow \mathbb{R}$ , where  $D \subseteq \mathbb{R}^2$  is some domain. We can interpret  $f$  as a scalar field over  $D$ . Take for example the temperature distribution or the height profile in a geometric map. Let us assume that the function  $f$  is not given explicitly, but only at certain points  $p_1, \dots, p_n \in D$  and we would like to compute  $f(p)$  for some arbitrary  $p \in D$ . In other words, we would like to interpolate  $f$ . In the following we denote by  $y_i$  the value associated to  $p_i$ .

From section 4.4.1 we recall that a piecewise linear function is a simple solution to this problem. However, in contrast to fig. 4.3a we now we deal with a piecewise linear surface as function graph of  $f$ . In fact, an even simpler solution would be a piecewise constant interpolation, a two-dimensional step function in some sense, but here again we would need to associate to each

point  $p_i$  a neighborhood to which we assign the value  $y_i$ . For both approaches, the piecewise constant and the piecewise linear interpolation, we can use the Voronoi diagram resp. the Delaunay triangulation.

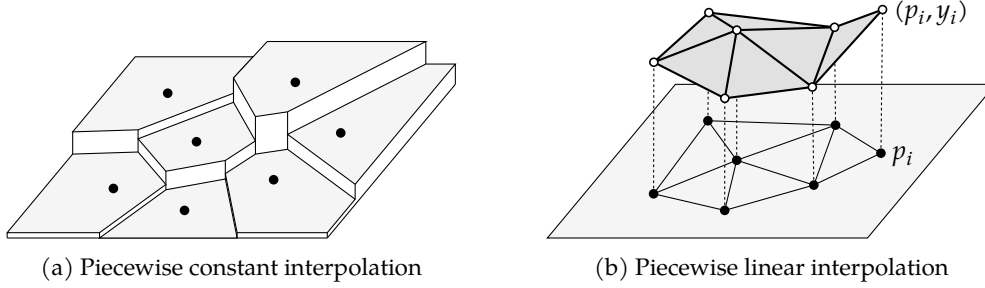


Figure 9.7: Approximating a function  $f: D \rightarrow \mathbb{R}$  over a domain  $D \subset \mathbb{R}^2$  given at a point set  $P = \{p_1, \dots, p_n\}$  with function values  $y_1, \dots, y_n$ . Left: A piecewise constant interpolation by computing  $V(P)$  and lifting each Voronoi region  $VR(p_i)$  by  $y_i$ . Right: A piecewise linear interpolation by computing  $D(P)$  and lifting each triangle vertex  $p_i$  by  $y_i$ .

**Piecewise constant interpolation.** For any  $p \in D$  we assign some function value of the set  $\{y_1, \dots, y_n\}$ . The most natural choice is probably to find the nearest neighbor  $p_i$  of  $p$  as the best representation among  $\{p_1, \dots, p_n\}$  and then take  $y_i$  as function value of  $p$ . So what we effectively do is that we assign the function value  $y_i$  to the entire Voronoi region  $VR(p_i)$  and so we receive a function graph as in fig. 9.7a.

This simple scheme also works if the co-domain of  $f$  is not  $\mathbb{R}$ , but any discrete set  $L$ , e.g., a set of labels. We therefore want to interpolate a function  $f: D \rightarrow L$  with a domain  $D \subseteq \mathbb{R}^2$  and a co-domain  $L$ . The idea of “classifying” a point  $p$  by its nearest neighbor  $p_i$  is exactly what the k-NN (k-nearest neighbor) classification algorithm in machine learning does for  $k = 1$ . Actually, there are generalizations of Voronoi diagrams to so-called *higher-order Voronoi diagrams* that are in exact correspondence to the k-NN classification algorithm for  $k \geq 1$ .

**Piecewise linear interpolation.** The piecewise constant interpolation is not continuous. For many applications, in order to compute an interpolation  $f(p)$  at a point  $p$  we would probably like to mix multiple function values  $y_i$  depending on the distance of  $p$  to  $p_i$ . So what we can do is to compute  $D(P)$  and lift each triangle vertex  $p_i$  by  $y_i$ . This gives as a continuous, triangulated surface as function graph, see fig. 9.7b.

Let us take any  $p$  in the domain  $D$ . We then project  $p$  vertically to the function graph to determine its interpolated function value  $f(p)$ . So if  $p$  is in the Delaunay triangle  $(p_1, p_2, p_3)$  then the function value of  $p$  is a mix of  $y_1, y_2$  and  $y_3$ . More precisely,  $p$  is then a convex combination

$$p = \lambda_1 p_1 + \lambda_2 p_2 + \lambda_3 p_3.$$

The coefficients  $\lambda_1, \lambda_2, \lambda_3$  are called the *Barycentric coordinates* of  $p$  (with respect to the affine basis  $p_1, p_2, p_3$ ). The function value assigned to  $p$  is simply

$$f(p) = \lambda_1 f(p_1) + \lambda_2 f(p_2) + \lambda_3 f(p_3) = \lambda_1 y_1 + \lambda_2 y_2 + \lambda_3 y_3,$$

which is now a convex combination of the function values  $y_1, y_2, y_3$ . Any triangulation would work for this method of constructing a piecewise linear interpolation. However, as the Delaunay

triangulation contains triangles that tend to be more equilateral, the (maximum) distance of a point  $p$  to its triangle vertices tend to be smaller. (The circumcenter of acute triangles is within the triangle.) Take for instance a point in the middle but slightly above the edge  $\overline{s_1s_4}$  in fig. 9.5b. Then such a point is better interpolated using the Delaunay triangulation at the right.

### 9.3.2 Euclidean MST and TSP

We could directly compute the EMST using, say, Kruskal's algorithm for the computation of the MST of arbitrary edge-weighted graphs applied to the complete Euclidean graph. Unfortunately, we would need to consider  $e = \binom{n}{2} = \frac{n(n-1)}{2}$  edges between all pairs of points and Kruskal's algorithm has a time complexity of  $O(e \log e)$ .

However, we can be shown that the EMST is part of the Delaunay triangulation, see fig. 9.8. We already know that the Delaunay triangulation has only a linear number of edges and can be computed in  $O(n \log n)$  time. Hence, we can compute the EMST in  $O(n \log n)$  time.

The ETSP problem is NP-hard, so there are no polynomial time algorithms assuming  $P \neq NP$ . However, one can use the EMST to compute so-called constant-factor approximations that are no worse than a factor of  $c > 1$  longer than the ETSP solution. Christofides' heuristic, for instance, computes a 1.5-approximation in  $O(n^3)$  time. In 2010 Aroa and Mitchell received the Gödel Prize for their independent discovery of (families of) polynomial-time algorithms that compute approximations for arbitrarily small  $c > 1$ . They discovered so-called *polynomial-time approximation schemes* (PTAS) for ETSP.

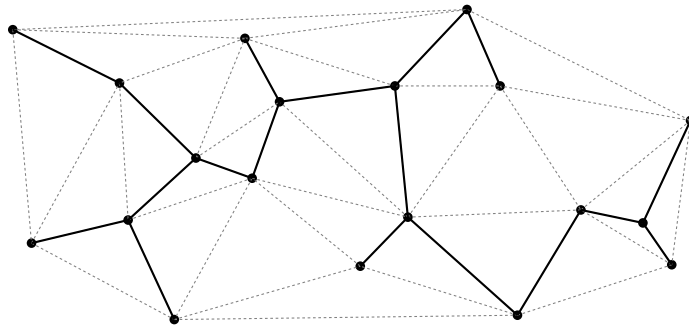


Figure 9.8: The Delaunay triangulation (dotted) contains the Euclidean minimum spanning tree (solid).

# Skeleton structures

## 10.1 Motivation

We denote by a *polygon with holes* a set  $P \subset \mathbb{R}^2$  that results from a polygon after removing polygons (holes) and we assume the holes do not reach the outer boundary of the original polygon. A polygon with holes,  $P$ , could model a two-dimensional terrain of a mobile disk-shaped robot  $V$ , or  $P$  could model a workpiece and  $V$  is an NC tool. On such polygons with holes we will introduce the notion of *skeleton structures* that will allow us to solve the following exemplary problems:

- First, we could ask whether  $V$  could reach a certain target position  $q \in P$  without leaving  $P$ . We interpret the boundary of  $P$  as walls.
- The diameter of  $V$  could be too large to pass through certain corridors of  $P$ . So a very related task would be to identify the so-called *bottlenecks* of  $P$ .
- Computing paths within  $P$  leads us to the desire to represent  $P$  as a transportation network, i.e., a graph structure consisting of nodes and edges. So another related goal is to transform the geometric shape  $P$  into a network structure.
- When we interpret  $P$  also as a workpiece that should be milled out by an NC machine or a garden that should be mowed. In either case we would like to compute a tool path for the CNC machine or the mowing robot.

## 10.2 Medial axis

The *medial axis*  $M(P)$  of a polygon with holes,  $P$ , consists of all points  $p \in P$  with the property that the largest disk within  $P$  and centered at  $p$  touches the boundary of  $P$  at two or more points. Put in different words,  $M(P)$  consists of all points  $p \in P$  that do not have a unique closest point to the boundary of  $P$ , see fig. 10.1.

We can actually interpret  $M(P)$  as a *transformation* that contracts the shape  $P$  to a 1-dimensional version while still somehow capturing topological features of  $P$ . For instance, every “loop” in  $P$  corresponds to “loop” in  $M(P)$ . But also if  $P$  resembles the shape of a hand with five fingers then  $M(P)$  contains a path for each finger. This is why the medial axis – also known as *medial axis transform* (MAT) – is widely known in the image processing domain for shape description, reconstruction and comparison.

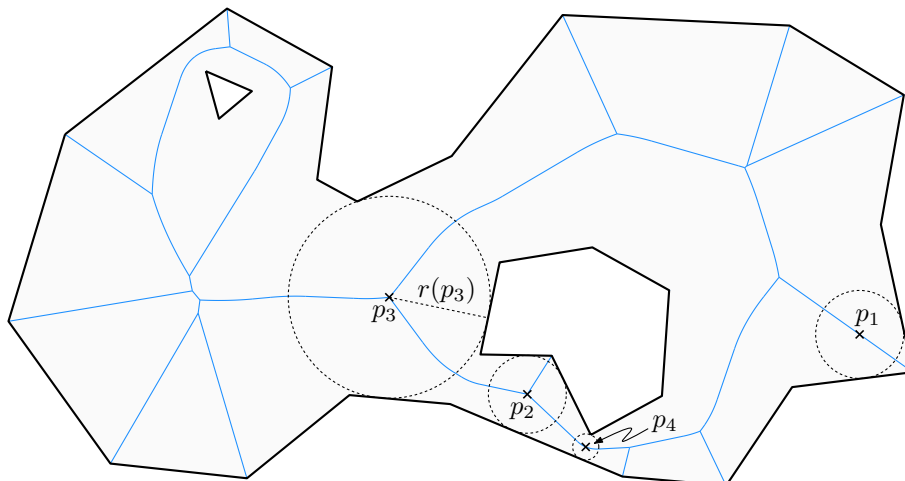


Figure 10.1: The medial axis  $M(P)$  in blue of a polygon with holes  $P$  shaded in gray. For some points  $p_i$  the disk  $D(p_i, r(p_i))$  with clearance radius  $r(p_i)$  is shown in dashed lines. The point  $p_4$  constitutes a bottleneck.

**Shape reconstruction.** The application for *shape reconstruction* stems from the following observation: Assume we do not know  $P$ , but we know  $M(P)$  and for each  $p \in M(P)$  we know the distance  $r(p)$  to the boundary of  $P$ . In fact, we interpret  $r$  as a function  $r: M(P) \rightarrow \mathbb{R}$  and call  $r(p)$  the *clearance radius* at  $p$ , see fig. 10.1. Then we can reconstruct  $P$  by

$$P = \bigcup_{p \in M(P)} D(p, r(p)), \quad (10.1)$$

where  $D(p, r(p))$  denotes the disk centered at  $p$  and with radius  $r(p)$ . That is, if we place at each  $p \in M(P)$  a disk of radius  $r(p)$  and build the union of those disks then we obtain  $P$  again. In this sense, eq. (10.1) is the inverse transformation of the medial axis transformation. We could exploit eq. (10.1) to modify the shape  $P$  by modifying  $r(p)$ , e.g., making certain “corridors” slimmer or wider by reducing or increasing  $r(p)$  at those points  $p \in M(P)$ . In some sense we edit the geometry of the shape but we leave the topology as is. Of course, if we change  $r(p)$  by too much then the topology of the resulting shape changes, e.g., holes may get filled up or bays may turn into cavities or bridges may disrupt.

**Bottlenecks.** Intuitively, a bottleneck is a narrow place of a corridor of  $P$ , a location where the boundary lines of  $P$  come close. The medial axis  $M(P)$  allows us to turn this intuitive description into a mathematical precise definition: A point  $p \in M(P)$  is called a *bottleneck* if  $p$  is a local minimum of the function  $r: M(P) \rightarrow \mathbb{R}$  as shown in fig. 10.1.

Note that a *minimum* of  $r$  is a place  $p \in M(P)$  with the following property: There is a small neighborhood around  $p$  such that for any point  $p'$  in this neighborhood  $r(p') \geq r(p)$  holds. In more details, there is a  $\varepsilon > 0$  such that for any  $p' \in M(P)$  with  $d(p, p') < \varepsilon$  it holds that  $r(p') \geq r(p)$ . Here  $d$  refers to the Euclidean distance<sup>1</sup>.

<sup>1</sup>It actually does not matter so much which distance (metric) we take but which topology the metric induces.

## 10.3 Generalized Voronoi diagrams

### 10.3.1 Introduction

The medial axis is a useful tool in computational geometry, so the practical question arises how to actually compute it. It turns out that the medial axis  $M(P)$  is actually part of a more general structure, namely the generalized Voronoi diagram  $V(P)$  of a polygon with holes  $P$ .

In section 9.1.1 we introduced the Voronoi diagrams of a point set in the Euclidean plane as a nearest-neighbor cell decomposition. We can generalize this idea from a point set to a more general set  $S$  of *sites*. The Voronoi diagram  $V(S)$  of the site set  $S$  is then called a *generalized Voronoi diagram*. There are other ways to generalize the Voronoi diagram of points, e.g., by generalizing the metric of the Euclidean plane or by considering cells defined by  $k$  nearest neighbors instead of one. But here we focus on generalized sites.

### 10.3.2 Straight-line segments and circular arcs

In industrial practice, we are particularly interested in points and straight-line segments and circular arcs. So let us denote by  $S$  a finite set of sites consisting of points, straight-line segments and circular arcs. To overcome some technical complications, we assume that for each straight-line segment or circular arc  $s \in S$  also both its endpoints are individual sites in  $S$ .

In fig. 10.2 we illustrate the Voronoi diagram as a nearest-neighbor cell decomposition of the plane that results from a straight-line segment and its endpoint and likewise for the circular arc. Mathematically, a point  $q$  in the Voronoi cell in an endpoint of  $s$  is just as close to the endpoint as to  $s$  itself. So in order to have a line-like Voronoi edge – with zero area – we have to perform a little exercise by introducing the concept of *cone of influence*  $I(s)$  of a site  $s$ . The idea is to restrict the Voronoi region  $VR(s)$  of a site  $s$  to a certain region, its cone of influence  $I(s)$ . The cone of influence is illustrated in fig. 10.2 and defined as follows:

$$I(s) = \begin{cases} \mathbb{R}^2 & \text{if } s \text{ is a point} \\ \text{orthogonal strip spanned by } s & \text{if } s \text{ is a straight-line segment} \\ \text{cone spanned by } s & \text{if } s \text{ is a circular arc} \end{cases}$$

A different way to define  $I(s)$  for straight-line segments or circular arcs  $s$  is by means of an intersection of two half spaces: At each end point of  $s$  we place a half space that contains  $s$  such that  $s$  is locally orthogonal to the boundary of the half space.

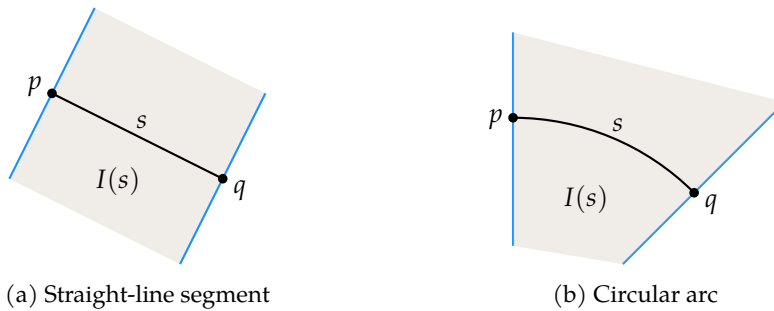


Figure 10.2: The Voronoi diagram of a straight-line segment  $s$  and its endpoints  $p, q$  and likewise for the circular arc. The Voronoi region  $VR(s)$  of  $s$  is restricted to its cone of influence  $I(s)$ .

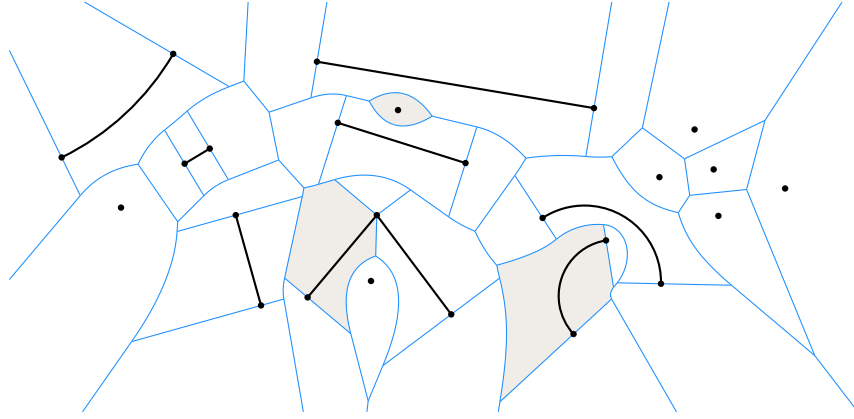


Figure 10.3: The generalized Voronoi diagram of points, straight-line segments and circular arcs. A few Voronoi regions are shaded in gray.

So now we can more or less copy over the definition of Voronoi diagram of points, see section 9.1.1, to the more general setting:

$$V(S) = \bigcup_{s \in S} VP(s) \quad (10.2)$$

where  $VP(s)$  is the Voronoi “polygon” and defined as the boundary  $\partial VR(s)$  of the Voronoi region  $VR(s)$ , which again is defined as

$$VR(s) = \{p \in I(s) : d(p, s) \leq d(p, s') \ \forall s' \in S\}. \quad (10.3)$$

Figure 10.3 shows the generalized Voronoi diagram of a couple of sites. A few Voronoi regions have been shaded in gray and form the nearest-neighbor cells of the respective sites.

A few remarks regarding the definition of the generalized Voronoi diagram are in order. By  $d(p, s)$  we mean the *infimum distance* between  $p$  and  $s$ , which means that

$$d(p, s) = \inf_{q \in s} d(p, q).$$

In fig. 10.4 we illustrate what this means in general: Roughly speaking,  $d(p, A)$  for a point  $p$  and a point set  $A$  is the smallest distance possible between  $p$  and any point  $q \in A$ . The very same idea could be generalized to the infimum distance  $d(A, B)$  between two point sets  $A$  and  $B$  of the plane.

There is a technical catch in eq. (10.3) which we ignored so far: For circular arcs  $s$  the definition in eq. (10.3) can cause irregularities in  $VR(s)$  in form of line-like needles attached to the “region body”. For instance, the point  $p$  in fig. 10.5 would be member of both Voronoi regions  $VR(s)$  and  $VR(s')$ , and so is the entire line segment to the circle center. Hence, the Voronoi polygons are no longer closed curves. In order to remove these irregularities, the definition of  $VR(s)$

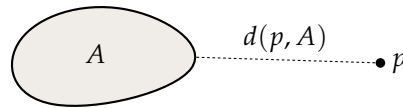


Figure 10.4: The infimum distance  $d(p, A)$  between a point  $p$  and a point set  $A$ .



is adapted to

$$VR(s) = \text{cl}\{p \in \text{int} I(s) : d(p, s) \leq d(p, s') \ \forall s' \in S\}, \quad (10.4)$$

which means that we first take the topological interior and then form the topological closure.<sup>2</sup> In simple words, the boundary of  $I(s)$  is first removed, which cuts off the needles, and then the boundary of the resulting set – the intended Voronoi polygon, a closed curve – is re-added. Details can be found in [16, 15].

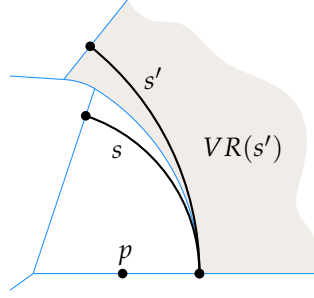


Figure 10.5: The point  $p \in VR(s)$ . But since  $d(p, s) = d(p, s')$  the point  $p$  would also be part of  $VR(s')$  if we would use eq. (10.3) instead of eq. (10.4).

### 10.3.3 Polygon with holes

Let us consider a polygon with holes  $P$ . Its boundary consists of vertices and edges. Let us denote by  $S$  the set of vertices and straight-line edges of  $P$ . We then define the Voronoi diagram  $V(P)$  of  $P$  simply as  $V(S)$ . Depending on the application and the context we may restrict the Voronoi diagram to  $P$  and ignore everything outside  $P$ .

In fig. 10.6 we show the Voronoi diagram  $V(P)$  of the same polygon with holes  $P$  as in fig. 10.1. We realize that they are essentially the same. More precisely,  $M(P) \subseteq V(P)$  and  $V(P) \setminus M(P)$  only consists of the Voronoi edges incident to reflex<sup>3</sup> vertices of  $P$ . This makes sense if we remember that  $M(P)$  consists of all points that have two nearest points on the boundary of  $P$ . These points therefore lie on the bisector between vertices and edges of  $P$  and no other site can be closer, so they must also lie on Voronoi edges. Hence, one way to compute the medial axis is to compute the Voronoi diagram and drop the Voronoi edges incident to reflex vertices.

Both, the concept of the medial axis and the concept of generalized Voronoi diagrams can be applied to polygons with holes, where the boundary elements are not only straight-line segments but also circular arcs. For industrial applications, especially in the CAD/CAM domain, this is of high relevance.<sup>4</sup>

<sup>2</sup>In topology we call  $O(c, r) = \{p \in \mathbb{R}^2 : \|p - c\| < r\}$  an open disk centered at  $c \in \mathbb{R}^2$  and with radius  $r$ . For a set  $A$  we define its interior,  $\text{int } A$ , as the set of points  $p \in A$  for which we can find a small enough  $r > 0$  such that  $D(p, r) \subseteq A$ . The closure  $\text{cl } A$  is defined by  $(\text{int } A^c)^c$ , where  $A^c = \mathbb{R}^2 \setminus A$  is the complement of  $A$ . The boundary of  $\partial A$  is defined as  $\text{cl } A \setminus \text{int } A$ .

<sup>3</sup>A reflex vertex is a non-convex vertex.

<sup>4</sup>In theory, the class of shapes  $P$  for which  $M(P)$  and  $V(P)$  have meaning can be extended to a significantly more general class.

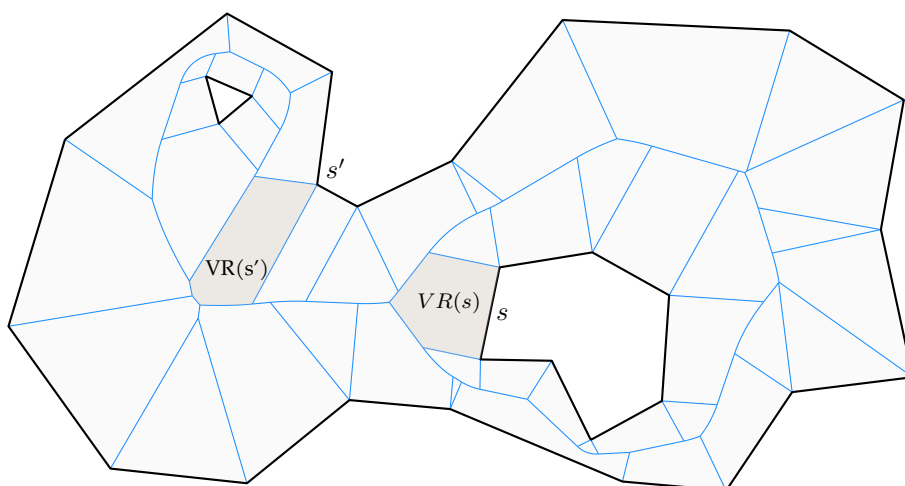


Figure 10.6: The Voronoi diagram  $V(P)$  of a polygon with holes  $P$  gives a nearest-neighbor cell decomposition of  $P$ . A few cells (Voronoi regions) are shaded in gray. The Voronoi diagram contains the medial axis  $M(P)$ , cf. fig. 10.1.

### 10.3.4 Computing generalized Voronoi diagrams

**Geometry.** If the site set  $S$  consists of points only then the Voronoi polygons  $VP(s)$  form convex polygons. In particular, the Voronoi edges are all straight-line edges and the reason for this is that Voronoi edges are sections of the bisector between two point sites.

For the generalized Voronoi diagram we now have to also take into account the bisector between all combinations of points, straight-line segments and circular arcs. A point can be seen as a circle with zero radius. It turns out that all bisectors are formed by conic sections.

- The bisector between a straight line and a circle is a parabola.
- The bisector between two circles is either a hyperbola or an ellipse.
- The bisector between two straight lines is a straight line.

The Voronoi nodes are located at the intersection of these bisectors. Directly computing the intersection of conic sections is not recommended from a numerical point of view. However, their location can also be computed by determining the points that are equidistant to three sites. This can actually be done by solving quadratic equations after the problem is transformed in an adequate way, see [16] for details.

**Topology.** The topology-oriented randomized incremental construction algorithm for Voronoi diagrams of points can be generalized to the generalized Voronoi diagram of points, straight-line segments and circular arcs. It can be proven that the expected runtime of the above algorithm is in  $O(n \log n)$ , see [15].

However, in order for that to work we require that when we insert a new site and therefore remove parts of the old Voronoi diagram then we only remove a tree structure, without cycles. This is actually not the case if we do not carefully prepare Voronoi edges: We need to split Voronoi edges at their apex (as conic sections). This means the following: If we consider the distance of points on the Voronoi edge to its two sites then this distance, in general, does not

change monotonically when sliding along the Voronoi edge. At the point on the Voronoi edge where this distance attains a minimum, we split the Voronoi edge and add a degree-2 Voronoi node. A detailed discussion on this procedure can be found in [16].

## 10.4 The grassfire model, offsetting and tool paths

Consider a point set  $S$  with  $n$  points in the plane and spread a grassfire at each of them. Assume the fire expands with equal speed in each direction, like circular waves that are emanated from the points in  $S$ . At certain locations in the plane the “fire waves” emanated from different points of  $S$  meet each other and the fire stops. What we receive is the picture in fig. 10.7: The points where the fires meet are exactly given by the Voronoi diagram  $V(S)$ .

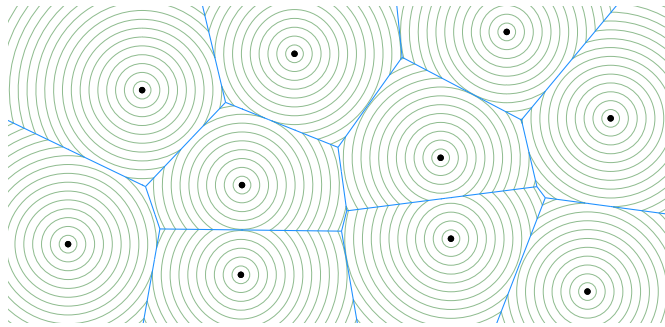


Figure 10.7: Grassfire model for a point set  $S$ . It sends out unit-speed offset waves from the sites in  $S$  and they interfere on  $V(S)$ .

Hence, we could actually define  $V(S)$  also as the “interference pattern” of isotropic unit-speed waves wavefronts. We can apply the very same idea not only to point sets  $S$ . In fig. 10.8 we illustrate the grassfire wavefronts emanated by the points and straight-line segments of a polygon with holes  $P$ . The interference patterns give as  $V(P)$  again.

In CAD/CAM we call these grassfire wavefronts “offset curves” and in geographic information systems we call this operation “buffering”. In NC-machining, wavefront curves are used for tool radius correction and the computation of tool paths, e.g., for NC milling machines or 3D plotters. Once the Voronoi diagram  $V(P)$  has been computed, an offset curve is computed in an easy, fast and numerically stable way by traversing the Voronoi diagram.

## 10.5 Straight skeletons

We call  $V(P)$  and  $M(P)$  a *skeleton* of  $P$  because it encodes topological features of  $P$ . In particular, for each hole of  $P$  we receive a cycle in the skeleton. They also encode certain geometric features, but a different skeleton would possibly encode different geometric features.

The grassfire model associated to Voronoi diagrams emanates a circular wavefront from non-convex vertices of a polygon with holes  $P$ , cf. fig. 10.8. What happens if we would emanate mitered offset curves instead? That is, the wavefront emanated at non-convex vertices would remain a sharp v-shape. So only the edges of  $P$  move inwards at unit speed and in parallel. Of course, the skeleton structure associated to this wavefront is different to  $V(P)$ . It is called the *straight skeleton*  $S(P)$ . Unlike the generalized Voronoi diagram, the straight skeleton consists of straight-line segments only, hence its name.

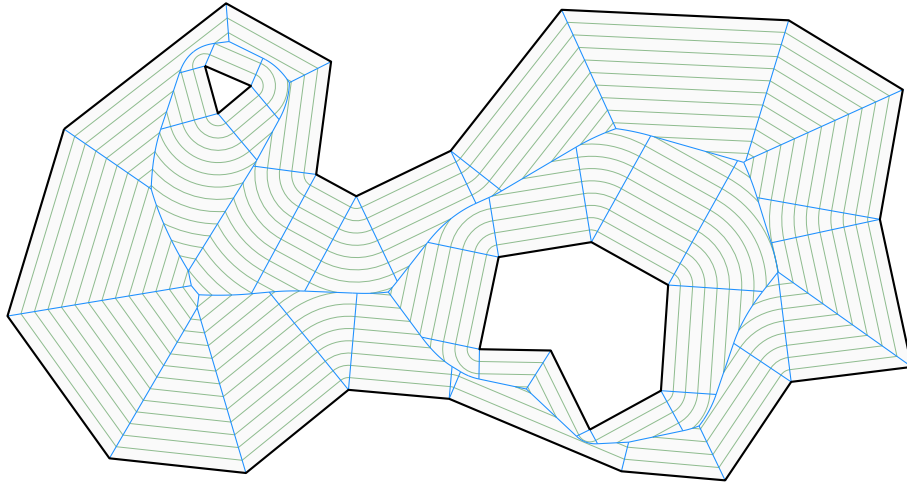


Figure 10.8: The offset curves given by grassfire wavefront curves. Its interference patterns create the Voronoi diagram.

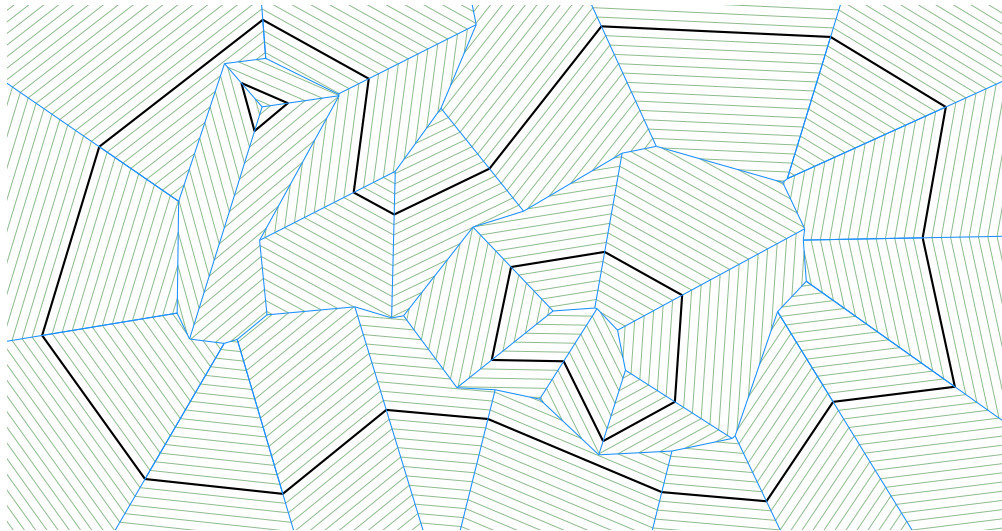


Figure 10.9: Mitered offset curves and the straight skeleton  $S(P)$  of a polygon with holes  $P$ .

# **Part IV**

## **Appendices**



## Selected details

### A.1 Computing cubic splines

In order to compute a natural cubic spline we could simply solve the linear equation system formed by the  $4(n-1)$  conditions in section 4.4.2.

If we take a closer look, however, we see that this system can be significantly simplified. First of all we apply a parameter substitution that in away shift and stretch the  $p_i$  such that they are defined over  $[0, 1]$  rather than  $[x_i, x_{i+1}]$ . More precisely, let

$$q_i(x) = p_i\left(\frac{x + x_i}{x_{i+1} - x_i}\right)$$

Hence,  $q_i(0) = p_i(x_i)$  and  $q_i(1) = p_i(x_{i+1})$ . If we know the  $q_i$  then we know the  $p_i$ , and vice versa.

The  $q_i$  are again polynomials

$$q_i(x) = a_i + b_i x + c_i x^2 + d_i x^3$$

Because  $a_i = q_i(0) = p_i(x_i) = y_i$  we immediately know that  $a_i = y_i$  and therefore

$$q_i(x) = y_i + b_i x + c_i x^2 + d_i x^3$$

$$q'_i(x) = b_i + 2c_i x + 3d_i x^2$$

$$q''_i(x) = 2c_i + 6d_i x$$

This leaves us with three unknowns  $b_i, c_i, d_i$  per polynomial. In the following we will use

$$q_i(1) = y_i + b_i + c_i + d_i$$

$$q'_i(1) = b_i + 2c_i + 3d_i$$

$$q'_i(0) = b_i$$

Note that  $q_i(1) = y_{i+1}$  and  $q'_i(1) = q'_{i+1}(0)$ , which gives us the system

$$y_i + b_i + c_i + d_i = y_{i+1}$$

$$b_i + 2c_i + 3d_i = b_{i+1}$$

We can solve for  $c_i$  and  $d_i$  and receive for  $1 \leq i \leq n-2$

$$c_i = 3(y_{i+1} - y_i) - 2b_i - b_{i+1}$$

$$d_i = 2(y_i - y_{i+1}) + b_i + b_{i+1}$$

If we know the  $b_i$  then we can compute the  $c_i$  and  $d_i$  and are done. So all unknowns that remain are  $b_1, \dots, b_{n-1}$ . What we did not use so far is that the second derivatives have to match too, i.e.,  $q_i''(1) = q_{i+1}''(0)$ . This gives for  $1 \leq i \leq n-3$

$$\begin{aligned} 2c_i + 6d_i &= 2c_{i+1} \\ c_i + 3d_i &= c_{i+1} \\ 3(y_{i+1} - y_i) - 2b_i - b_{i+1} + 6(y_i - y_{i+1}) + 3b_i + 3b_{i+1} &= 3(y_{i+2} - y_{i+1}) - 2b_{i+1} - b_{i+2} \\ b_i + 4b_{i+1} + b_{i+2} &= 3(y_{i+2} - y_i) \end{aligned}$$

For a natural spline we also require  $q_1''(0) = q_{n-1}''(1) = 0$ . This gives  $c_1 = 0$  and  $2c_{n-1} + 6d_{n-1} = 0$  and results after some calculations in the equations

$$\begin{aligned} 2b_1 + b_2 &= 3(y_2 - y_1) \\ b_{n-2} + 2b_{n-1} &= 3(y_n - y_{n-1}) \end{aligned}$$

Altogether we end up with  $n-1$  equations for  $b_1, \dots, b_{n-1}$ :

$$\begin{pmatrix} 2 & 1 & & & \\ 1 & 4 & 1 & & \\ & 1 & 4 & 1 & \\ & & 1 & 4 & 1 \\ & & & \ddots & \\ & & & 1 & 4 & 1 \\ & & & & 1 & 2 \end{pmatrix} \cdot \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ \vdots \\ b_{n-2} \\ b_{n-1} \end{pmatrix} = \begin{pmatrix} 3(y_2 - y_1) \\ 3(y_3 - y_1) \\ 3(y_4 - y_2) \\ 3(y_5 - y_3) \\ \vdots \\ 3(y_n - y_{n-2}) \\ 3(y_n - y_{n-1}) \end{pmatrix}$$

The coefficient matrix is a so-called *tridiagonal* matrix. Such equation systems can be actually solved in  $O(n)$  time by dedicated algorithms. See [21] for details. Solving the linear system gives us the  $b_i$ , which then yield  $c_i$  and  $d_i$ , after which we know the polynomials  $q_i$ . These can then be transformed back to the  $p_i$  if desired.

## A.2 Proof sketch for in-circle point location

In section 5.2.5 we learned about a determinate in eq. (5.5) that allows for location tests of points  $p$  for circles given by three points  $a, b, c$ . What follows is a proof sketch.

Let us consider the case where  $\odot(a, b, c, p) = 0$ . The determinant is zero when the fourth row of the determinant is a linear combination of the other three rows, i.e.,

$$\begin{pmatrix} p_x \\ p_y \\ p_x^2 + p_y^2 \\ 1 \end{pmatrix} = \alpha \begin{pmatrix} a_x \\ a_y \\ a_x^2 + a_y^2 \\ 1 \end{pmatrix} + \beta \begin{pmatrix} b_x \\ b_y \\ b_x^2 + b_y^2 \\ 1 \end{pmatrix} + \gamma \begin{pmatrix} c_x \\ c_y \\ c_x^2 + c_y^2 \\ 1 \end{pmatrix}.$$

for some coefficients  $\alpha, \beta, \gamma$ . We can reinterpret this equation as three equations

$$\begin{aligned} 1 &= \alpha + \beta + \gamma \\ p &= \alpha a + \beta b + \gamma c \\ \|p\|^2 &= \alpha \|a\|^2 + \beta \|b\|^2 + \gamma \|c\|^2 \end{aligned}$$



The first two lines say that  $\alpha, \beta, \gamma$  are coefficients of an affine combination, namely  $p$  is an affine combination of the three points  $a, b, c$ . Let us denote by  $m \in \mathbb{R}^2$  the center and by  $r$  the radius of the circumcircle of  $a, b, c$ . Then we can rephrase the third equation as follows

$$\begin{aligned}
\|p\|^2 &= \alpha\|a\|^2 + \beta\|b\|^2 + \gamma\|c\|^2 \\
\|p\|^2 + \|m\|^2 &= \alpha(\|a\|^2 + \|m\|^2) + \beta(\|b\|^2 + \|m\|^2) + \gamma(\|c\|^2 + \|m\|^2) \\
\|p\|^2 + \|m\|^2 - 2p \cdot m &= \alpha(\|a\|^2 + \|m\|^2 - 2a \cdot m) + \beta(\|b\|^2 + \|m\|^2 - 2b \cdot m) + \gamma(\|c\|^2 + \|m\|^2 - 2c \cdot m) \\
(\|p - m\|)^2 &= \alpha(\|a - m\|)^2 + \beta(\|b - m\|)^2 + \gamma(\|c - m\|)^2 \\
(\|p - m\|)^2 &= r^2.
\end{aligned}$$

Note that we used  $r = \|a - m\| = \|b - m\| = \|c - m\|$  and  $p \cdot m = (\alpha a + \beta b + \gamma c) \cdot m$ . This fourth equation is therefore equivalent to saying  $p$  is on the circle and  $\odot(a, b, c, p)$  is zero on the circumcircle of  $a, b, c$ . Within the circle and outside the circle it is either entirely positive or entirely negative as  $\odot(a, b, c, p)$  is continuous in  $p$ . However, note that  $\odot(a, b, c, p)$  tends towards  $\infty$  when  $p$  goes to infinity because the co-factor

$$\begin{vmatrix} a_x & a_y & 1 \\ b_x & b_y & 1 \\ c_x & c_y & 1 \end{vmatrix}$$

of  $\odot(a, b, c, p)$  is positive for counterclockwise  $a, b, c$ . Hence,  $\odot(a, b, c, p)$  is positive everywhere outside the circle (and negative inside).



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