

Introduction to Numerical Linear Algebra

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At Trier University variants of this course serve the modules:

- Elements of Mathematics
- Elemente der Linearen Algebra
- Numerical Methods for Geoscientists



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A Short Note on Programming

...and specifically on Python.



Programming Languages in Numerical Mathematics (selection)

- **Fortran** (FORmula TRANslation) (1957):
 - proprietary (e.g. from IBM) and free compilers
 - intended for numerical calculations (matrix and vector operations)
 - extensive libraries
 - LAPACK (**L**inear **A**lgebra **P**ackage) standard library for numerical linear algebra
- **C** (1972)/ **C++** (1985):
 - universal programming language
 - Standard libraries for numerics: Armadillo, LAPACK++ (based on LAPACK)
- **MATLAB** (MATrrix LABoratory) (1984):
 - proprietary software from MathWorks
 - designed for numerical mathematics (matrix and vector operations)
- **Mathematica** (1988):
 - proprietary software from Wolfram Research
 - visualization of 2d/3d objects
 - symbolic processing of equations
 - see also: <https://www.wolframalpha.com/>
- **Python** (1990): open source
 - universal programming language (several application areas)
 - for numerical calculations: SciPy (2001), NumPy (1995,2006), matplotlib (2003).
- **Julia** (2012): open source
 - developed mainly for scientific computing
 - syntax looks like MATLAB
 - execution speed is in the range of C and Fortran

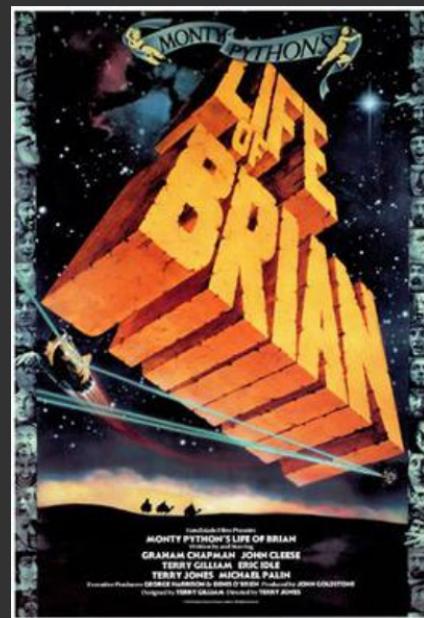
→ All programming related parts of this lecture will be presented and implemented using **Python 3**

Why Python?

- universal, multi-purpose programming language
 - many packages for scientific computing, web development, ...
- open source and free (Python Software Foundation License (PSFL), OSI/FSF approved)
- multi-platform (runs on all operating systems)
- design philosophy: easy syntax, readable code (almost looks like pseudocode)
- Also see: <https://www.youtube.com/watch?v=M0vBoBqqjr0>

Background

- developed in 1990 by Guido van Rossum (Netherlands)
 - name is homage to Monty Python
- interpreter (scripting) programming language
(≠ compiled language such as C or Fortran)
- used by: Google Mail, Google Maps, YouTube, Dropbox, sphinx, and many more
- for scientific computing we use from the Scipy Stack:
 - **NumPy** (1995,2006)
 - **SciPy** (2001)
 - **matplotlib** (2003)



Programming Workflow

CLI [ex:demo]

- Any text editor can be used (emacs, vi, vim, nano, geany, gedit,...)
 - many editors provide syntax highlighting
- Install Python and then interpret the source code

IDE [ex:demo]

- For software development it is often more convenient to use an **integrated development environment (IDE)**
- Specifically for Python:  PyCharm¹,  Spyder

¹sign up to jetbrains with your university account and you can get the PyCharm professional edition!

For exercise submission/presentation:



Jupyter-Notebook [ex:demo]

- open source, *web based* interactive environment
→ thus multi-platform
- developed by **Project Jupyter** (NPO)
→ name refers to: **Julia, Python, R**
- the whole process can be documented:
Coding → Documentation → Run → Communication and Presentation
- in fact, a jupyter notebook contains all the input **and** output of an interactive session plus additional text
→ complete record!
- client VS server
 - client (local lightweight machine): browser-based workflow
 - server (remote, number cruncher): does the actual computation

Get Started



- We recommend to download the distribution *Anaconda*:

<https://www.anaconda.com/distribution/>

→ available for Linux, Windows, and MacOS

- Comes along with:
 - graphical user interface (*Anaconda Navigator*)
 - Spyder, Jupyter Notebook, RStudio (IDE for R)
 - installs all important packages (NumPy, SciPy, matplotlib, TensorFlow, scikit-learn, \$\\dots\$)
 - package manager (*Conda*) (standard is *pip*)

Tutorials

- Scientific computing with Python:
<https://scipy-lectures.org/>
- Official Online-Documentation:
<https://docs.python.org/3/>
- Official Python Tutorial:
<https://docs.python.org/3/tutorial/index.html>
- Quickstart to Jupyter Notebook:
<https://jupyter.readthedocs.io/en/latest/content-quickstart.html>

Final remark:

- For Software development I would always go with an IDE due to the many additional tools: debugging, variable explorer, version control, file manager, etc.
- However, Jupyter Notebooks are very well suited for presentations and thus teaching. In particular for mandatory submissions, since the tutor can see your output, even if the program does not run on his/her machine (for whatever reasons).

A Short Introduction to the Topic

From the Module Handbook:

*"After completing the module, the students know the mathematical foundations in the areas of linear algebra and **numerical mathematics**. As part of the course, they acquire or deepen knowledge in the programming language **Python**."*

Numerical mathematics?

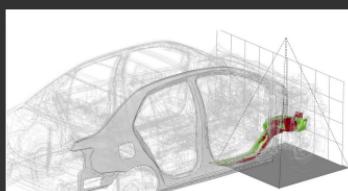
From Wikipedia: Field of mathematics that deals with the construction and analysis of algorithms to approximately (but accurately) compute solutions to (hard) continuous problems – typically using computers.

Why is this important?

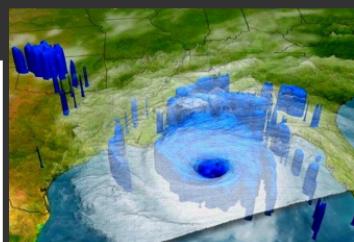
- most (all?) **application**-oriented problems cannot be solved exactly → **hard** problems



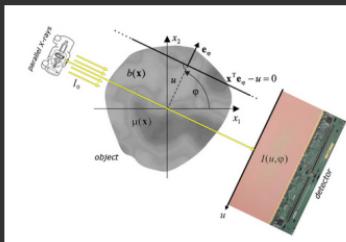
trajectories of objects in
space
2020SO



car crash simulation



weather prediction



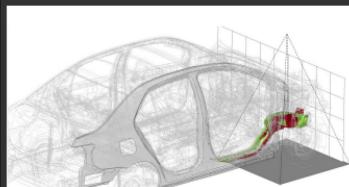
CT Scan

Relation to Data Science?

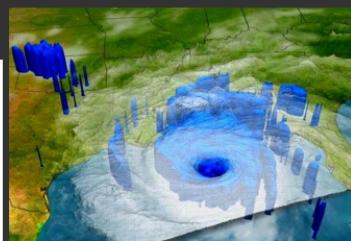
- due to the high amount of data available **data-driven** models are more important than ever
- data can be considered as a **mathematical object** (e.g., as a matrix/vector)
- with **numerical algorithms** we can manipulate data:
 - solve systems involving the data (fitting data, prediction,...)
 - extract the most important features (singular values, PCA, data compression,...)
 - calibrate models against data (machine learning, neural networks,...)



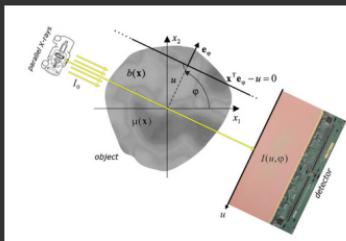
trajectories of objects in
space
2020SO



car crash simulation



weather prediction



CT Scan

Preview

Let us assume we have m data points

$$(z_i, y_i), \quad i = 1, \dots, m,$$

where

- z_i are n -dimensional vectors of *explanatory features*
- y_i are k -dimensional vectors representing the *response/prediction/classification*

→ *The term “vector” already indicates that Linear Algebra comes naturally into the game.*

Examples

- You ask m persons about

$$z_i = (\text{age, sex, weight, height, years of experience}) \quad (n = 5 \text{ dimensional vector})$$

$$y_i = \text{salary} \quad (k = 1 \text{ dimensional vector})$$

- Consider m years where

$$z_i = \text{year} \quad (n = 1 \text{ dimensional vector})$$

$$y_i = \text{global mean temperature} \quad (k = 1 \text{ dimensional vector})$$

- Consider m images that you want to classify

$$z_i = (p_{lj})_{lj} \quad (\text{image stored as matrix/vector})$$

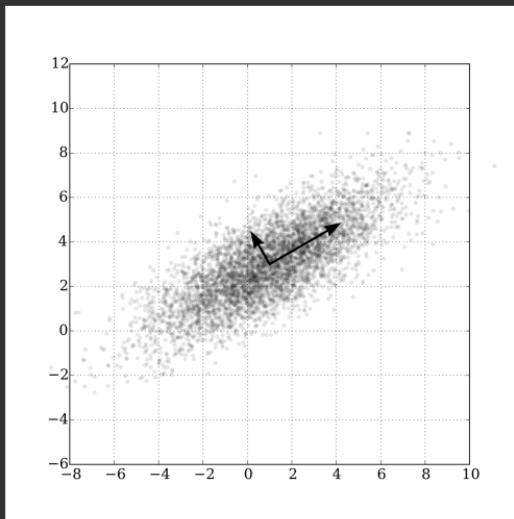
$$y_i = (\text{dog, cat, elephant}) \quad (k = 3 \text{ dimensional vector})$$

Dealing solely with the features z

Applications of the **Singular Value Decomposition** are:

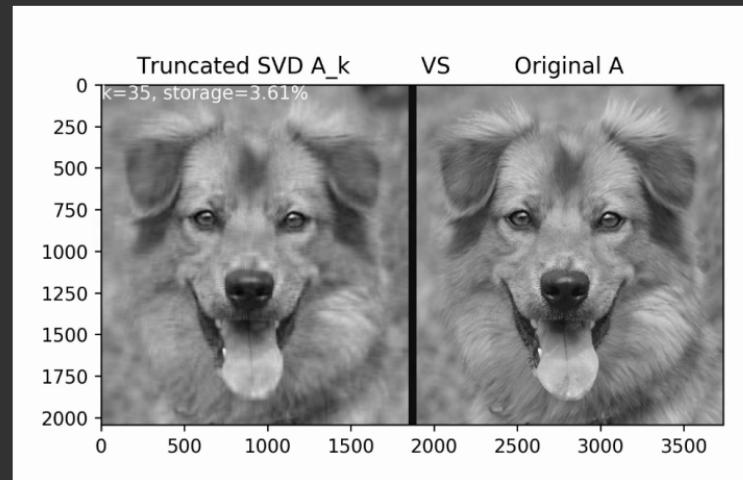
Principal Component Analysis (PCA)

→ Aim: dimension reduction



Data compression

→ Aim: compression without dimension reduction



Relating features z to response y

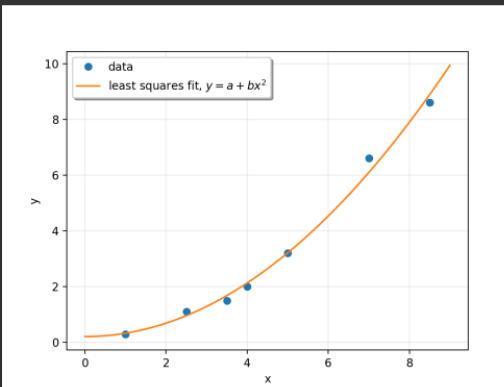
One central goal in many scientific fields is to find a **model** f_x depending on some parameters $x = (x_i)_i$, which “best” explains the relation between z_i and y_i in the sense that

$$f_x(z_i) \approx y_i, \quad \text{for all } i = 1, \dots, m$$

- **The task:** Find those parameters x for which the “distance” between our prediction $f_x(z_i)$ and the measured response y_i is “as small as possible”.
- Math gives us the tools to rigorously define this task, to analyze it systematically and to provide numerical solutions!

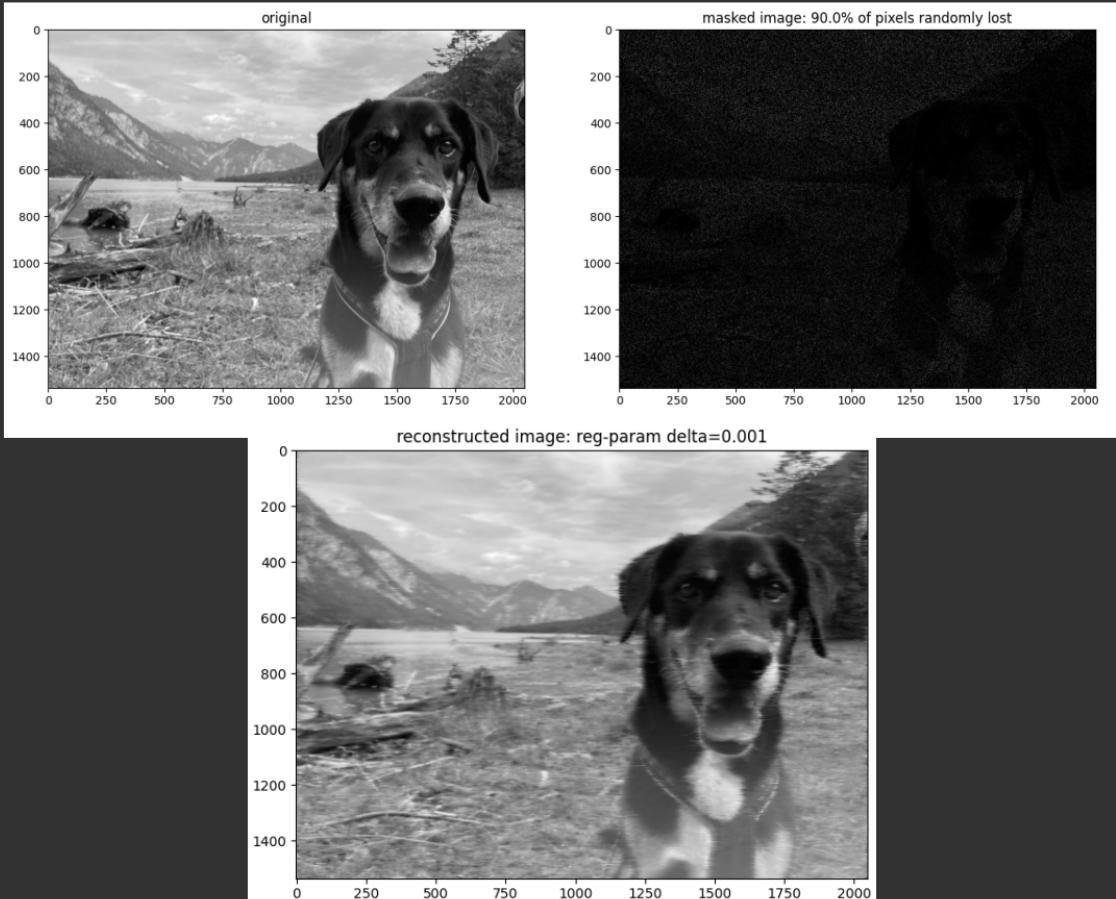
Curve Fitting

$$f_x(z) := x_0 + x_1 z + x_2 z^2$$



Simple image inpainting

$$\min_x \|Ax - b\|^2 + R(x)$$



Take away message

Math provides a rigorous framework of abstract structures (Definition) within which their properties and relations (Theorem) can be systematically analyzed (Proof).

The same mathematical concept can be exploited in multiple applications; see, e.g., SVD above.

Given a real-world problem the user has to provide an interface (a mathematical model) to these concepts to make use of the mathematical theory.

Math Basics

0 Mathematical Basics

In this first section we will provide mathematical notations and concepts which are fundamental and crucial for the further presentation.

0.1 Statements

By a **statement** we mean a linguistic or mental construction that is either true or false.

Example 0.1

- “4 is an even number.” is a true statement.
- “Bananas have conic shape.” is a false statement.
- “In the night, it is colder than outside.” is not a statement.
- “There are infinitely many stars.” is a statement, which can be true or false.

Relations and Operations

$\neg A$: *A is false (**negation**)*

$A \Rightarrow B$: *from A follows B; if A is true, then also B is true (**implication**)*

*we say: A is **sufficient** for B, B is **necessary** for A*

$A \Leftrightarrow B$: *A is true, if and only if B is true. (**equivalence**)*

Note that the following two statements are equivalent

$$A \Rightarrow B$$

$$\neg B \Rightarrow \neg A$$

For example A : “it rains”, B : “the street is wet”, then $\neg A$: ... and $\neg B$: ...

0.2 Sets

Definition 0.2 (Set) According to Cantor a *set* is a well-defined collection of distinct objects, considered as an object in its own right. The objects that make up a set (also known as the set's *elements*) can be anything: numbers, people, letters of the alphabet, other sets, and so on.

Notation: curly brackets $\{\}$

Example 0.3

- $M := \{1, 2, 3\}$
- $N := \{ \underbrace{x}_{\text{element}} \mid \underbrace{x \text{ is multiple of } 7}_{\text{element property}} \} = \{x : x \text{ is multiple of } 7\} = \{7, 14, 21, \dots\}$

→ Note: We use “ $:=$ ” for definitions

Definition 0.4 (Cardinality) If a set M is *finite* (i.e., it only contains finitely many elements), then we denote by $|M|$ the number of elements contained in M and call it *cardinality of M* .

Set relations and further definitions

$a \in M$ (or $M \ni a$): a is element of M ; M contains a

$a \notin M$ (or $M \not\ni a$): a is not element of M ; M does not contain a

$M = \{1, 2, 3\}$, $1 \in M$, $\{1\} \notin M$

$M = N$: M contains the same elements as N

$M \neq N$: M does not contain the same elements as N

$N := \{1, 2\}$, $M = M$, $M \neq N$

$M \subset N$ (or $M \subseteq N$): M is subset of N , i.e., each element of M is also an element of N ; equality of sets is permitted.

$N \supset M$ (or $N \supseteq M$): N is superset of M ; analogously

$M \subsetneq N$: M is strict subset of N ; $M \neq N$

$\emptyset = \{\}$: empty set

$N \subset M$ and even $N \subsetneq M$; what about the relation between $N_2 := \{\{1\}, 2\}$ and M or \emptyset and M ?

Remark: Very useful in practice to show that two sets are equal:

$$M = N \iff M \subset N \text{ and } N \subset M$$

$\mathcal{P}(M)$

power set of M defined by

$\mathcal{P}(M) := 2^M := \{N : N \subset M\}$ (set of all subsets of M)

We find $|\mathcal{P}(M)| = 2^{|M|}$

Let us consider $M = \{1, 2\}$, then $|M| = 2$ and the power set of M is given by

$$\mathcal{P}(M) = 2^M = \{\emptyset, \{1\}, \{2\}, \{1, 2\}\}.$$

We also find

$$|\mathcal{P}(M)| = 4 = 2^{|M|} = 2^2.$$

Remark: **Binomial theorem**

$$\sum_{k=0}^n \binom{n}{k} = 2^n,$$

where

$$\binom{n}{k} := \frac{n!}{k!(n-k)!}$$

is the so-called binomial coefficient, which give us the number of subsets with k elements that we can draw from a set with n elements.

Summary: Set relations and further definitions

$a \in M$ (or $M \ni a$):	a is element of M ; M contains a
$a \notin M$ (or $M \not\ni a$):	a is not element of M ; M does not contain a
$M = N$:	M contains the same elements as N
$M \neq N$:	M does not contain the same elements as N
$M \subset N$ (or $M \subseteq N$):	M is subset of N , i.e., each element of M is also an element of N ; equality of sets is permitted.
$N \supset M$ (or $N \supseteq M$):	N is superset of M ; analogously
$M \subsetneq N$:	M is strict subset of N ; $M \neq N$
$\emptyset = \{\}$:	empty set
$M \times N$:	Cartesian product defined by $M \times N := \{(m, n) : m \in M, n \in N\}$
	$M^n := M \times \dots \times M$ (n times)
$\mathcal{P}(M)$	power set of M defined by
	$\mathcal{P}(M) := 2^M := \{N : N \subset M\}$ (set of all subsets of M)
	We find $ \mathcal{P}(M) = 2^{ M }$

Set operations

$$M \cup N := \{a : a \in M \text{ or } a \in N\} \quad (\text{union})$$

$$M \cap N := \{a : a \in M \text{ and } a \in N\} \quad (\text{intersection})$$

$$M \setminus N := \{a : a \in M \text{ and } a \notin N\} \quad (\text{difference})$$

If $N \subset M$

$$N^c := \overline{N} := M \setminus N \quad (\text{complement of } N \text{ with respect to } M)$$

M, N are called **disjoint**, if $M \cap N = \emptyset$.

Example 0.5

Let $M = \{1, 2, 3, 4\}$ and $N = \{1, 3\}$, then

$$M \cup N = \{1, 2, 3, 4\}, \text{ we always have } M \subset M \cup N \text{ and } N \subset M \cup N$$

$$M \cap N = \{1, 3\}$$

$$\overline{N} = M \setminus N = \{2, 4\}$$

For combinations of those set operations we have the following result:

Lemma 0.6 (De Morgan's laws) Let Ω be a set and $M, N \subset \Omega$. Then we find

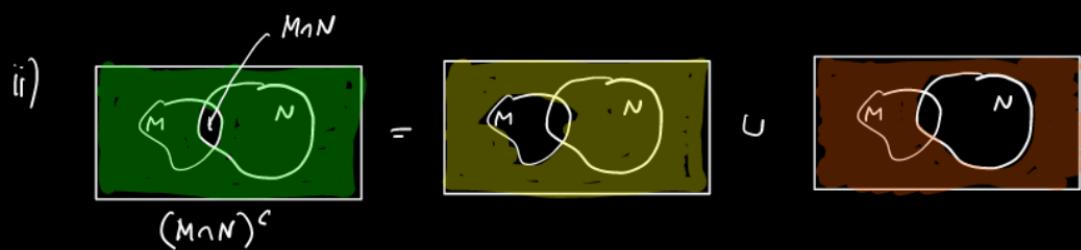
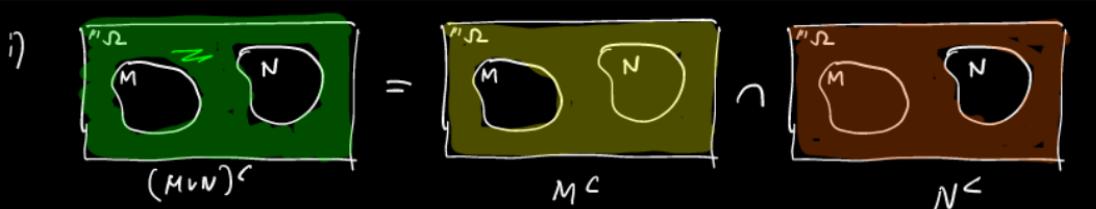
- i) $(M \cup N)^c = M^c \cap N^c$,
- ii) $(M \cap N)^c = M^c \cup N^c$.

Here the complements are taken with respect to Ω .

Proof. Exercise.

□

Illustration:



0.3 Functions

Definition 0.7 (function) Let M, N be two sets. A **function** or **mapping** f from M to N (notation: $f: M \rightarrow N$) is determined by

- its **domain** M ,
- its **codomain** N ,
- and a **rule**,

that uniquely assigns to each element $a \in M$ an $b := f(a) \in N$ (notation: $a \mapsto f(a)$).

Two functions $f_1 : M_1 \rightarrow N_1$ and $f_2 : M_2 \rightarrow N_2$ are called **equal** (abbr. $f_1 \equiv f_2$) (identical), if $M_1 = M_2$, $N_1 = N_2$ and $f_1(a) = f_2(a)$ for all $a \in M_1$ (i.e., equal, domain, codomain and rule).

Example 0.8

Let $M := N := \{1, 2, 3, 4, 5, \dots\}$ and consider $f: M \rightarrow N$, $a \mapsto 2a$. How could we “visualize” this function?

i) a **table** with two columns (one for domain and codomain each)

follow where points go from $A = \{1, 2\} \subset M$

find points which would produce $B = \{4, 6\} \subset N$

ii) draw the **graph** into a coordinate system

We introduce function related sets:

Definition 0.9 (Image, preimage, graph) Let $A \subset M$ and $B \subset N$, then

- i) the set $f(A) = \{f(a) : a \in A\} \subset N$ is called **image set** of A (under f),
- ii) the set $f^{-1}(B) = \{a \in M : f(a) \in B\} \subset M$ is called **preimage** of B (under f),
- iii) the set $\text{graph}(f) := \{(a, f(a)) : a \in M\} \subset M \times N$ is called the **graph** of f .

→ **Attention:** Here, f^{-1} is not the inverse function (see below).

– [abstract picture with with image, preimage and graph]

– With the definitions from above we have

for $A = \{1, 2\}$ we find $f(A) = \{2, 4\}$

for $B = \{4, 6\}$ we find $f^{-1}(B) = \{2, 3\}$

$\text{graph}(f) = \{(1, 2), (2, 4), (3, 6), \dots\}$

Important properties of functions:

Definition 0.10 (Injective, surjective, bijective) A function $f : M \rightarrow N$ is called

- i) **injective (one-to-one)**, if $f(a) \neq f(\tilde{a})$ for all $a, \tilde{a} \in M$ with $a \neq \tilde{a}$;
- ii) **surjective (onto)**, if for all $b \in N$ there exists an $a \in M$ with $f(a) = b$ (or equivalently $f(M) = N$);
- iii) **bijective**, if f is injective as well as surjective relation.

We can invert bijective functions:

Definition 0.11 (Inverse function) Let $f : M \rightarrow N$ be a bijective (invertible) function. Then there exists a (unique) function $f^{-1} : N \rightarrow M$, the so-called **inverse of f** , such that

$$f(a) = b \iff f^{-1}(b) = a.$$

Example 0.12 Consider again example from above and the visualization with the help of the table.

We can concatenated two or more functions:

Definition 0.13 (Composition) Let $f: M \rightarrow N$ and $g: N \rightarrow P$ be functions, then we call the function

$$g \circ f: M \rightarrow P, a \mapsto g(f(a))$$

composition of f and g .

- [abstract picture for composition of the functions
- Concrete example:

$$M = \{1, 2, 3, 4, \dots\}, N := \{x : x \text{ is even}\}, P := \{x : x \text{ is odd}\},$$

$$f: M \rightarrow N, a \mapsto 2a, g: N \rightarrow P, b \mapsto b - 1$$

$$(g \circ f)(6) = g(\underbrace{f(6)}_{=12}) = g(12) = 12 - 1 = 11$$

A function with “no effect”:

Definition 0.14 (Identity function) Let M be a set. Then the function

$$id := id_M: M \rightarrow M, a \mapsto a$$

is called the **identity function on M** .

0.4 Numbers

The notion of **number** has been extended over the centuries, here we do not go in detail through the axiomatic construction but just point out some properties that are useful in the remaining.

Here is an overview:

\mathbb{N}	Natural	$\{1, 2, 3, 4, 5, \dots\}$	counting objects order relation: $m \leq n$ $m + n, m \cdot n$ proof concept of induction
\mathbb{Z}	Integer	$\{\dots, -3, -2, -1, 0, 1, 2, 3, \dots\}$	adding zero and negative numbers (borrowing money,...) $(\mathbb{Z}, +)$ ordered, commutative group
\mathbb{Q}	Rational	$\left\{ \frac{p}{q} : p, q \in \mathbb{Z}, q \neq 0 \right\}$	adding fractions of objects (one half of a cake) $(\mathbb{Q}, +, \cdot)$ ordered field
\mathbb{R}	Real	$\mathbb{Q} \cup \{\text{limits of sequences in } \mathbb{Q}\}$	adding square roots ($\sqrt{2}, \sqrt{5}, \dots$), π, \dots $(\mathbb{R}, +, \cdot)$ ordered and complete field
\mathbb{C}	Complex	$\{a + ib : a, b \in \mathbb{R}\}, i := \sqrt{-1}$	adding e.g. square root of negative numbers $\mathbb{R} \times \mathbb{R}$ with a special multiplication $(\mathbb{C}, +, \cdot)$ complete field (not ordered)

We have

$$\mathbb{N} \subsetneq \mathbb{Z} \subsetneq \mathbb{Q} \subsetneq \mathbb{R} \subsetneq \mathbb{C}$$

0.4.1 Complex Numbers \mathbb{C}

$\mathbb{C} = \text{"}\mathbb{R} \times \mathbb{R} \text{ with a special multiplication"}$

- extension: e.g., imaginary unit $i := \sqrt{-1}, \sqrt{-3}, \dots$
- in real life: electricity and roots of polynomials (e.g., which do not touch the x -axis)

Definition 0.15 (Complex numbers \mathbb{C}) We define the field of complex numbers $(\mathbb{C}, +, \cdot)$ by $\mathbb{C} := \mathbb{R} \times \mathbb{R}$ with the binary operations

$$\begin{aligned}+ &: (a_1, b_1) + (a_2, b_2) := (a_1 + a_2, b_1 + b_2), \\ \cdot &: (a_1, b_1) \cdot (a_2, b_2) := (a_1 a_2 - b_1 b_2, a_1 b_2 + a_2 b_1).\end{aligned}$$

Note that \mathbb{R} itself is identified with $\mathbb{R} \times \{0\} \subset \mathbb{C}$.

Remarks

- the product in \mathbb{C} is all the magic
- $(\mathbb{C}, +, \cdot)$ is a (*complete*) **field**
- as a 2-dimensional object, \mathbb{C} does **not** possess an order relation

In order to alleviate the memorizing of the product definition, it is customary to use the so-called **imaginary unit** $i := \sqrt{-1}$ and perform computations as if it would be a real number:

For $z = (a_1, b_1)$, $w = (a_2, b_2) \in \mathbb{C}$ we write

$$z = a_1 + ib_1 \text{ and } w = a_2 + ib_2.$$

Then the product naturally computes as

$$z \cdot w = (a_1 + ib_1) \cdot (a_2 + ib_2) = a_1a_2 + ib_1a_2 + ia_1b_2 + \underbrace{i^2}_{-1} b_1b_2 = (a_1a_2 - b_1b_2) + i(a_1b_2 + a_2b_1).$$

Example 0.16

$$z \in \mathbb{C} : z = a + ib$$

$$(1 + 2i) \cdot (3 + 4i) = 3 + 4i + 6i + 8i^2 = 3 + 10i - 8 = -5 + 10i$$

$$\frac{1 + 2i}{3 + 4i} = \frac{(1 + 2i)(3 - 4i)}{(3 + 4i)(3 - 4i)} = \frac{3 - 4i + 6i - 8i^2}{9 + 16} = \frac{11 + 2i}{25}$$

[note on real and imaginary part, complex conjugate]

In \mathbb{C} every non-constant polynomial has at least one root in \mathbb{C} (we say \mathbb{C} is *algebraically closed*):

Theorem 0.17 (Fundamental theorem of algebra) Let $\alpha_0, \alpha_1, \dots, \alpha_n \in \mathbb{C}$ with $n \geq 1$, $\alpha_n \neq 0$ (i.e., nonzero leading coefficient) and consider the nonconstant polynomial $p: \mathbb{C} \rightarrow \mathbb{C}$,

$$p(z) := \sum_{i=0}^n \alpha_i z^i.$$

Then, there are numbers $\lambda_1, \dots, \lambda_n \in \mathbb{C}$ such that

$$p(z) = \alpha_n \prod_{i=1}^n (z - \lambda_i) = \alpha_n \cdot (z - \lambda_1) \cdot \dots \cdot (z - \lambda_n), \quad \forall z \in \mathbb{C}.$$

In particular, the λ_i are precisely the roots of p , i.e., $p(\lambda_i) = 0$ for $i = 1, \dots, n$.

Example 0.18

Consider the polynomial $p: \mathbb{C} \rightarrow \mathbb{C}$, $p(z) := z^2 + 1$.

What are the roots of p ?

$$0 = p(z) = z^2 + 1 \Leftrightarrow z^2 = -1 \Leftrightarrow z \in \{i, -i\}$$

We find

$$p(z) = (z - i)(z + i) \quad (= z^2 + 1)$$

The polynomial p has no roots considered as a function $\mathbb{R} \rightarrow \mathbb{R}$, but exactly two roots as a function $\mathbb{C} \rightarrow \mathbb{C}$

0.4.2 Summary

$$\mathbb{N} \subsetneq \mathbb{Z} \subsetneq \mathbb{Q} \subsetneq \mathbb{R} \subsetneq \mathbb{C}$$

\mathbb{N}	Natural	$\{(0), 1, 2, 3, \dots\}$	order relation
\mathbb{Z}	Integer	$\{\dots, -3, -2, -1, 0, 1, 2, 3, \dots\}$	$(\mathbb{Z}, +)$ ordered, commutative group
\mathbb{Q}	Rational	$\left\{ \frac{p}{q} : p, q \in \mathbb{Z}, q \neq 0 \right\}$	$(\mathbb{Q}, +, \cdot)$ ordered field
\mathbb{R}	Real	$\mathbb{Q} \cup \{\text{limits of sequences in } \mathbb{Q}\}$	$(\mathbb{R}, +, \cdot)$ ordered and complete field
\mathbb{C}	Complex	$\{a + ib : a, b \in \mathbb{R}\}, i := \sqrt{-1}$	$(\mathbb{C}, +, \cdot)$ algebraically closed field

Most **theoretical** investigations deal with real numbers $r \in \mathbb{R}$.

Numerical computations can only be performed with *floating point numbers* (short: *floats*) with a relative error (typically 10^{-16}) in each operation.

Many of the following results hold for general fields, say $(\mathbb{F}, +, \cdot)$. However the only fields we will know about are the real numbers \mathbb{R} and the complex numbers \mathbb{C} ; thus we always think of $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$.

0.5 Sequences

Numerical methods often produce sequences which (in the best case) *converge* to a desired solution. Also besides this, the concept of a limiting process to *infinity* is the basis for many other notions in mathematics (differentiation/integration/...).

For simplicity, in the following we only consider sequences in \mathbb{R} . In order to have a notion of “distance” we will consider the metric

$$d: \mathbb{R} \times \mathbb{R} \rightarrow [0, +\infty), \quad d(x, y) := |x - y|,$$

where

$$|x| := \text{abs}(x) := \begin{cases} x, & \text{if } x \geq 0 \\ -x, & \text{else} \end{cases} \quad (\text{absolute value of } x).$$

In the following, \mathbb{R} can also be replaced by any set X which can be equipped with a so-called **metric** d (in math we call (X, d) a metric space).

Example 0.19 Consider the set

$$\left\{ \frac{1}{2}, \frac{1}{4}, \frac{1}{8}, \dots \right\} = \left\{ \left(\frac{1}{2} \right)^k : k \in \mathbb{N} \right\} = \{x(k) : k \in \mathbb{N}\}$$

What happens for large k ? Also have a look at the graph.

We introduce the notion of sequence and some important related properties:

Definition 0.20 (Sequence) Let M be a set. Then a function $x: \mathbb{N} \rightarrow M$ is called a **sequence**.

Notation: $(x^k)_{k \in \mathbb{N}}$, $\{x^k\}_{k \in \mathbb{N}}$ or $\{x^k\}_{k=1}^\infty$.

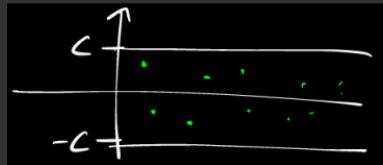
Example 0.21 Let $a \in \mathbb{R}$.

- i) The **constant sequence** $\{a\}_{k \in \mathbb{N}}$, i.e., $x^k := a$ for $k \in \mathbb{N}$ trivially converges to $\bar{x} := a$.
- ii) The sequence $\{\frac{1}{k}\}_{k \in \mathbb{N}}$, i.e., $x^k := \frac{1}{k}$ for $k \in \mathbb{N}$ is a null sequence, since it converges to $\bar{x} := 0$.
- iii) The sequence $\{a + \frac{1}{k}\}_{k \in \mathbb{N}}$, i.e., $x^k := a + \frac{1}{k}$ converges to $\bar{x} := a$.
- iv) The sequence $\{a \cdot \frac{1}{k}\}_{k \in \mathbb{N}}$, i.e., $x^k := a \cdot \frac{1}{k}$ converges to $\bar{x} := 0$.
- v) The **alternating sequence** $\{a(-1)^k\}_{k \in \mathbb{N}}$, i.e., $x^k := a(-1)^k$ does not converge.

Definition 0.22 Let $(x^k)_{k \in \mathbb{N}}$ be a sequence in \mathbb{R} . Then $(x^k)_{k \in \mathbb{N}}$ is called

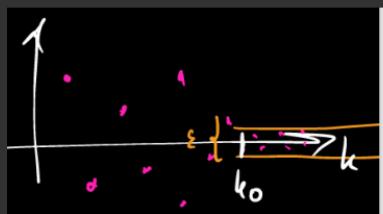
- i) **bounded**, if there exists a uniform bound $C > 0$ such that for all $k \in \mathbb{N}$

$$d(x^k, 0) = |x^k| \leq C.$$



- ii) **Cauchy**, if for any $\varepsilon > 0$ there is a $k_0 \in \mathbb{N}$ such that for all $m, n \geq k_0$

$$d(x^m, x^n) = |x^m - x^n| < \varepsilon.$$



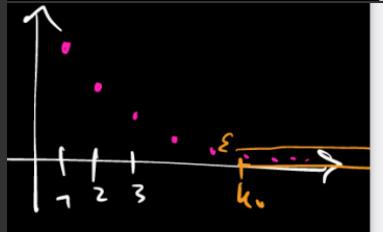
- iii) **null sequence**, if for any $\varepsilon > 0$ there is a $k_0 \in \mathbb{N}$ such that for all $k \geq k_0$

$$d(x^k, 0) = |x^k| < \varepsilon.$$

We write $\lim_{k \rightarrow \infty} x^k = 0$.

- iv) **convergent**, if there exists a $\bar{x} \in \mathbb{R}$ such that $(x^k - \bar{x})_{k \in \mathbb{N}}$ is a null sequence, i.e., $\lim_{k \rightarrow \infty} (x^k - \bar{x}) = 0$.

We write $\lim_{k \rightarrow \infty} x^k = \bar{x}$.



- v) **divergent**, if it does not converge.

Example 0.23 Let $a \in \mathbb{R}$. The following sequences are bounded:

- i) The constant sequence $\{a\}_{k \in \mathbb{N}}$ (choose $C = a$),
- ii) The sequence $\{\frac{1}{k}\}_{k \in \mathbb{N}}$ (choose $C = 1$),
- iii) The alternating sequence $\{a(-1)^k\}_{k \in \mathbb{N}}$ (choose $C = a$). This sequence is not convergent but bounded.

An example of an unbounded sequence is given by

- iv) the sequence $\{k^2\}_{k \in \mathbb{N}}$.

Theorem 0.24 (Uniqueness of limits) Let $(x^k)_{k \in \mathbb{N}}$ be a sequence in \mathbb{R} , then $(x^k)_{k \in \mathbb{N}}$ has at most one limit.

Proof. We proof the statement by contradiction. Therefore, let us assume $(x^k)_{k \in \mathbb{N}}$ converges to \bar{x}_1 and \bar{x}_2 , with $\bar{x}_1 \neq \bar{x}_2$. We define $\varepsilon := \frac{1}{2}|\bar{x}_1 - \bar{x}_2| > 0$. Then by definition of the limit there exist $N_1 \in \mathbb{N}$ and $N_2 \in \mathbb{N}$ so that

$$|x^k - \bar{x}_1| < \varepsilon \text{ and } |x^k - \bar{x}_2| < \varepsilon$$

for all $k \geq \max\{N_1, N_2\}$. Thus, by triangle inequality it follows

$$2\varepsilon = |\bar{x}_1 - \bar{x}_2| = |\bar{x}_1 - (x^k - x^k) - \bar{x}_2| \leq |\bar{x}_1 - x^k| + |x^k - \bar{x}_2| < 2\varepsilon.$$

Since $2\varepsilon < 2\varepsilon$ is a contraction for $\varepsilon > 0$, we have that there cannot exist two distinct limits \bar{x}_1 and \bar{x}_2 as assumed above. \square

Important relation between the different types of sequences:

Theorem 0.25 Let $(x^k)_{k \in \mathbb{N}}$ be a sequence in \mathbb{R} , then

$$(x^k)_{k \in \mathbb{N}} \text{ convergent} \Rightarrow (x^k)_{k \in \mathbb{N}} \text{ Cauchy} \Rightarrow (x^k)_{k \in \mathbb{N}} \text{ bounded.}$$

Proof. We only prove the first implication (the second implication requires some more technical steps). For this purpose let $\tilde{\varepsilon} > 0$. Since $(x^k)_{k \in \mathbb{N}}$ is a convergent sequence, there exists a $\bar{x} \in \mathbb{R}$ and a $k_0 \in \mathbb{N}$, so that

$$|x^m - \bar{x}| < \tilde{\varepsilon} \text{ and } |x^n - \bar{x}| < \tilde{\varepsilon}$$

for all $m, n \geq k_0$. Thus, by triangle inequality it follows that

$$|x^m - x^n| = |x^m - (\bar{x} - \bar{x}) + x^n| \leq |x^m - \bar{x}| + |x^n - \bar{x}| < 2\tilde{\varepsilon}.$$

Consequently, for $\varepsilon := \tilde{\varepsilon}/2$ we can choose the same k_0 to show the Cauchy property. \square

An important tool to compute limits in practice is the following:

Theorem 0.28 (Sums and products of sequences) Let $(x^k)_{k \in \mathbb{N}}$ and $(y^k)_{k \in \mathbb{N}}$ be two sequences in \mathbb{R} with $\lim_{k \rightarrow \infty} x^k = \bar{x}$ and $\lim_{k \rightarrow \infty} y^k = \bar{y}$. Then

- i) $\lim_{k \rightarrow \infty} (x^k + y^k) = \lim_{k \rightarrow \infty} x^k + \lim_{k \rightarrow \infty} y^k = \bar{x} + \bar{y};$
- ii) $\lim_{k \rightarrow \infty} (x^k \cdot y^k) = \lim_{k \rightarrow \infty} x^k \cdot \lim_{k \rightarrow \infty} y^k = \bar{x} \cdot \bar{y}.$

In particular we find for $a \in \mathbb{R}$ that $\lim_{k \rightarrow \infty} (x^k + a) = \bar{x} + a$ and $\lim_{k \rightarrow \infty} (x^k \cdot a) = \bar{x} \cdot a$.

Proof. i) We define $z^k := x^k + y^k$ and $\bar{z} := \bar{x} + \bar{y}$. Let $\varepsilon > 0$. For $\tilde{\varepsilon} := \varepsilon/2$ there exists a $k_0 \in \mathbb{N}$, so that

$$|x^k - \bar{x}| < \tilde{\varepsilon} \text{ and } |y^k - \bar{y}| < \tilde{\varepsilon}$$

for all $k \geq k_0$. Thus by triangle equality we find

$$\begin{aligned} |z^k - \bar{z}| &= |x^k + y^k - (\bar{x} + \bar{y})| = |x^k - \bar{x} + y^k - \bar{y}| \leq |x^k - \bar{x}| + |y^k - \bar{y}| \\ &< \tilde{\varepsilon} + \tilde{\varepsilon} = \varepsilon. \end{aligned}$$

ii) We define $z^k := x^k \cdot y^k$ and $\bar{z} := \bar{x} \cdot \bar{y}$. First note that by Theorem ??, we have that the sequence $(x^k)_{k \in \mathbb{N}}$ is bounded, which implies that there exists a bound $C > 0$ so that $|x^k| < C$ for all $k \in \mathbb{N}$. By triangle inequality, we find

$$\begin{aligned} |z^k - \bar{z}| &= |x^k y^k - \bar{x} \bar{y}| = |x^k y^k - (x^k \bar{y} - x^k \bar{y}) + \bar{x} \bar{y}| = |x^k(y^k - \bar{y}) + (x^k - \bar{x})\bar{y}| \\ &\leq |x^k(y^k - \bar{y})| + |(\bar{x} - x^k)\bar{y}| = |x^k|(|y^k - \bar{y}|) + |(\bar{x} - x^k)||\bar{y}| \leq C(|y^k - \bar{y}|) + |(\bar{x} - x^k)||\bar{y}|. \end{aligned} \tag{1}$$

Now let $\varepsilon > 0$. Then for $\tilde{\varepsilon} := \varepsilon/(C + |\bar{y}|) > 0$ there exists a $k_0 \in \mathbb{N}$, so that

$$|x^k - \bar{x}| < \tilde{\varepsilon} \text{ and } |y^k - \bar{y}| < \tilde{\varepsilon}$$

for all $k \geq k_0$. Thus, combining this with (??) gives the desired result

$$|z^k - \bar{z}| < C\tilde{\varepsilon} + \tilde{\varepsilon}|\bar{y}| = (C + |\bar{y}|)\tilde{\varepsilon} = \varepsilon.$$

□

Example 0.29 Let $a \in \mathbb{R}$.

- i) The sequence $\{a + \frac{1}{k}\}_{k \in \mathbb{N}}$
- ii) The sequence $\{a \cdot \frac{1}{k}\}_{k \in \mathbb{N}}$
- iii) The sequence $\{\frac{1}{k^2}\}_{k \in \mathbb{N}}$

Example 0.31 Let $f: \mathbb{N} \rightarrow \mathbb{N}$ with $f(k) \geq 0$ for all $k \in \mathbb{N}$. Then the sequence $\{\frac{1}{k+f(k)}\}_{k \in \mathbb{N}}$ is a null sequence.

0.6 Quadratic equations and completion of the square

We want to solve quadratic equations of the following kind

$$x^2 + px + q = 0, \quad (2)$$

where $p, q \in \mathbb{R}$ are fixed. Representation (??) is sometimes referred to as **normalized form** or **reduced form**.

Recall the binomial formulas: For $a, b \in \mathbb{R}$ we have

- i) $(a + b)^2 = a^2 + 2ab + b^2$
- ii) $(a - b)^2 = a^2 - 2ab + b^2$
- iii) $(a + b)(a - b) = a^2 - b^2$

Example 0.32 We want to find all $x \in \mathbb{R}$, that satisfy the quadratic equation

$$x^2 + 6x + 5 = 0.$$

In general we find:

If $\left(\frac{p}{2}\right)^2 \geq q$, then the quadratic equation

$$x^2 + px + q = 0$$

is solved by

$$x = -\frac{p}{2} \pm \sqrt{\left(\frac{p}{2}\right)^2 - q}.$$

Proof.

□

Alternative representation (I)

Quadratic equations are also often introduced in the following form:

$$ax^2 + bx + c = 0 \quad (3)$$

for fixed $a, b, c \in \mathbb{R}$. Representation (??) is referred to as the **general form** of a quadratic equation.

Assumed $a \neq 0$ we can deduce the reduced form (??):

Example 0.33 We want to find all $x \in \mathbb{R}$, that satisfy the quadratic equation

$$2x^2 + 8x + 6.72 = 0.$$

Alternative representation (II)

Quadratic equations are also introduced as:

$$a(x - h)^2 + k = 0 \quad (4)$$

for fixed $a, h, k \in \mathbb{R}$. Representation (??) is referred to as **vertex form**.

Again, we can deduce the reduced form:

Summary

0.7 Inequalities

Here we make use of the fact that \mathbb{R} is an ordered field. In particular we will exploit the **monotonicity** property:

Let $a, b \in \mathbb{R}$ with $a \leq b$. Then

- 1) $\forall c \in \mathbb{R}: a + c \leq b + c$;
- 2) $\forall c \geq 0: ac \leq bc$.

From 1) and 2) it follows that

$$\forall c < 0: ac \geq bc$$

Example 0.34 We want to find all $x \in \mathbb{R}$, that satisfy the inequality

$$x^2 + 6x + 5 \geq 0.$$

Example 0.35 We want to find all $x \in \mathbb{R}$, that satisfy the inequality

$$2x \geq 5x - 6.$$

Example 0.36 We want to find all $x \in \mathbb{R}$, that satisfy the inequality

$$\frac{x+4}{4x-12} \leq 2.$$

Fundamentals of Linear Algebra

Recommended reading for this section:

- Lectures 1,2,3 in [4]
- Sections I.1, I.2, I.3, I.5(, I.11) in [3]
- Chapters 1,3(,4,5) in [2]

Literature:

- [1] R. Rannacher.
Numerik 0 - Einführung in die Numerische Mathematik.
Heidelberg University Publishing, 2017.
- [2] G. Strang.
Introduction to Linear Algebra.
Wellesley-Cambridge Press, 2003.
- [3] G. Strang.
Linear Algebra and Learning from Data.
Wellesley-Cambridge Press, 2019.
- [4] L.N. Trefethen and D. Bau.
Numerical linear algebra.
SIAM, Soc. for Industrial and Applied Math., Philadelphia, 1997.

1 Fundamentals of Linear Algebra

1.1 Matrices and Vectors

Example 1.1 (*Interpolation*)

Assume we are given the following measurements

z_i	-1	0	1
y_i	0	1	0

We postulate that these measurements can be explained exactly by the (quadratic) model

$$f(z) := f_x(z) := x_1 + x_2 z^2.$$

Question: Can we find parameters $x_1, x_2 \in \mathbb{R}$, so that $f(z_i) = y_i$ for all $i = 1, \dots, 3$?

We first translate the task into the following system of *linear* equations:

$$\begin{array}{lcl} i=1 : & 1x_1 + 1x_2 & = 0 \\ i=2 : & 1x_1 + 0x_2 & = 1 \\ i=3 : & 1x_1 + 1x_2 & = 0 \end{array} \Leftrightarrow \underbrace{\begin{pmatrix} 1 & 1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix}}_A \cdot \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_x = \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}_b \Leftrightarrow Ax = b$$

Why linear? Roughly speaking, because the x_i only appear with power 1 and there are no combinations $x_i x_j$.

Also note, the abstracting notation $Ax = b$ provides a rigorous interface to analyze this problem theoretically and also to implement numerical solvers.

[ex:solve and draw points]

Throughout we will consider matrices over $\mathbb{F} \in \{\mathbb{R}, \mathbb{C}\}$. However, \mathbb{F} could be replaced by any **field**.

Definition 1.2 (Matrix)

Let $m, n \in \mathbb{N}$. Then a rectangular array of numbers in \mathbb{F} with m rows and n columns, written as

$$A = (a_{ij})_{ij} = \begin{pmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{pmatrix},$$

is called a $(m \times n)$ **matrix with coefficients in \mathbb{F}** .

$\mathbb{F}^{m \times n}$: set of all $(m \times n)$ matrices with coefficients in \mathbb{F}

$\mathbb{F}^n := \mathbb{F}^{n \times 1}$: matrices with just one column are called (column) "**vectors**"; elements in $\mathbb{F}^{1 \times n}$ are referred to as **row vectors**

a_{ij} : the (i, j) -th **coefficient or entry**

(a_{i1}, \dots, a_{in}) : the i -th **row** of A (this is a $(1 \times n)$ -matrix, , n -dimensional vector)

$\begin{pmatrix} a_{1j} \\ \vdots \\ a_{mj} \end{pmatrix}$: the j -th **column** of A (this is a $(m \times 1)$ -matrix, m -dimensional vector)

0 : the **zero matrix or null matrix**, i.e. all entries 0

I_n : the **unity or identity matrix** in $\mathbb{F}^{n \times n}$, i.e. the Matrix with entries

$$\delta_{ij} = \begin{cases} 1, & \text{if } i = j \\ 0, & \text{else} \end{cases} \quad (\text{"Kronecker delta"}, \quad \text{i.e.} \quad I_n = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix})$$

Operations

We can add matrices of same size and scale the entries of a matrix.

Example 1.3 (*Summing and scaling matrices*)

$$\begin{pmatrix} 2 & 1 \\ 0 & -1 \end{pmatrix} + \begin{pmatrix} 1 & -1 \\ 1 & 0 \end{pmatrix} := \begin{pmatrix} 3 & 0 \\ 1 & -1 \end{pmatrix}$$
$$2 \cdot \begin{pmatrix} 2 & 1 \\ 0 & -1 \end{pmatrix} = \begin{pmatrix} 2 \cdot 2 & 2 \cdot 1 \\ 2 \cdot 0 & 2 \cdot (-1) \end{pmatrix} := \begin{pmatrix} 4 & 2 \\ 0 & -2 \end{pmatrix}$$

Definition 1.4 (*Summing and scaling matrices*) Let $A, B \in \mathbb{F}^{m \times n}$ be matrices, $m, n \in \mathbb{N}$ and $r \in \mathbb{F}$.

i) **Sum of matrices:** $+: \mathbb{F}^{m \times n} \times \mathbb{F}^{m \times n} \rightarrow \mathbb{F}^{m \times n}$

The sum $C := A + B$ of the two matrices A and B is defined to be the matrix $C = (c_{ij})_{ij} \in \mathbb{F}^{m \times n}$ with entries

$$c_{ij} := a_{ij} + b_{ij} \quad \text{for } i = 1, \dots, m, j = 1, \dots, n.$$

ii) **Multiplication with scalars:** $\cdot: \mathbb{F} \times \mathbb{F}^{m \times n} \rightarrow \mathbb{F}^{m \times n}$

The product of the matrix A with $r \in \mathbb{F}$ is defined to be the scaled matrix

$$r \cdot A := (r \cdot a_{ij})_{ij}.$$

In this context, elements of the field \mathbb{F} are called **scalars**.

Question: How do summing and scaling get along in a mixed expression?

We can prove the following rules:

Lemma 1.5 (Compatibility properties of summing and scaling) Let $A, B \in \mathbb{F}^{m \times n}$ and $r, s \in \mathbb{F}$. Then

$$i) \quad (r \cdot s) \cdot A = r \cdot (s \cdot A)$$

$$ii) \quad (r + s) \cdot A = r \cdot A + s \cdot A$$

$$iii) \quad r \cdot (A + B) = r \cdot A + r \cdot B$$

$$iv) \quad 1 \cdot A = A$$

Proof. Follow immediately from Definition ?? in terms of matrix coefficients and the field properties of \mathbb{F} . For example:

$$i) \quad (r \cdot s)A = [(r \cdot s)a_{ij}]_{ij} \stackrel{\text{(associativity in } \mathbb{F})}{=} [r \cdot (s \cdot a_{ij})]_{ij} = r \cdot (s \cdot A)$$

$$ii) \quad (r + s)A = [(r + s)a_{ij}]_{ij} \stackrel{\text{(distributivity in } \mathbb{F})}{=} [ra_{ij} + sa_{ij}]_{ij} = r \cdot A + s \cdot A$$

□

Remark 1.6 One can show that $(\mathbb{F}^{m \times n}, +)$ is a so-called abelian group. Then the compatibility properties from Lemma ?? imply that $(\mathbb{F}^{m \times n}, +, \cdot)$ is a so-called vector space (over \mathbb{F}).

From Lemma ?? we can deduce further properties of $(\mathbb{F}^{m \times n}, +, \cdot)$.

Corollary 1.7 Let $A \in \mathbb{F}^{m \times n}$ and $r \in \mathbb{F}$. Then

$$i) \quad 0 \cdot A = 0$$

$$ii) \quad r \cdot 0 = 0$$

$$iii) \quad r \cdot A = 0 \Rightarrow r = 0 \vee A = 0$$

$$iv) \quad (-1) \cdot A = -A \quad (\text{i.e., } (-1) \cdot A \text{ is the additive inverse of } A)$$

Proof. Follows from Lemma ?? and the field properties of \mathbb{F} . For example:

iv) To show: $(-1) \cdot A + A = 0$. We find

$$(-1) \cdot A + A \stackrel{(\text{L.?? iii}))}{=} (-1) \cdot A + 1 \cdot A \stackrel{(\text{L.?? (ii)})}{=} (-1 + 1) \cdot A = 0 \cdot A \stackrel{(\text{i})}{=} 0.$$

Next we provide a notation which enables us to write linear systems of equations in a concise way.
We recall from Example ??:

$$\begin{array}{rcl} 1x_1 + 1x_2 & = & 0 \\ 1x_1 + 0x_2 & = & 1 \\ 1x_1 + 1x_2 & = & 0 \end{array} \Leftrightarrow: \underbrace{\begin{pmatrix} 1 & 1 \\ 1 & 0 \\ 1 & 1 \end{pmatrix}}_A \cdot \underbrace{\begin{pmatrix} x_1 \\ x_2 \end{pmatrix}}_x = \underbrace{\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix}}_b \Leftrightarrow Ax = b$$

Definition 1.8 (Matrix-Vector Product) Let $A \in \mathbb{F}^{m \times n}$ and $x \in \mathbb{F}^n$. Then the **matrix-vector product** $b = Ax \in \mathbb{F}^m$ is defined by

$$b_i = a_{i1}x_1 + a_{i2}x_2 + \dots + a_{in}x_n =: \sum_{\ell=1}^n a_{i\ell}x_\ell, \quad \forall i = 1, \dots, m.$$

A matrix $A \in \mathbb{F}^{m \times n}$ can therefore also be considered as a (linear) mapping

$$f_A : \mathbb{F}^n \rightarrow \mathbb{F}^m, \quad x \mapsto Ax.$$

Example 1.9 (Matrix-Vector Product)

Let us consider $A = \begin{pmatrix} 1 & 2 \\ 2 & 0 \\ 0 & 1 \end{pmatrix}$ with columns $a_1 = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}$ and $a_2 = \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix}$. Then

$$\begin{array}{l} i = 1 \\ i = 2 \\ i = 3 \end{array} \quad \begin{pmatrix} 1 & 2 \\ 2 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} 0.5 \\ 3 \end{pmatrix} = \begin{pmatrix} 1 \cdot 0.5 + 2 \cdot 3 \\ 2 \cdot 0.5 + 0 \cdot 3 \\ 0 \cdot 0.5 + 1 \cdot 3 \end{pmatrix} = \begin{pmatrix} 6.5 \\ 1 \\ 3 \end{pmatrix}.$$

There are two ways of perceiving the matrix-vector product:

(1) By rows: *Used for computations*

$$\begin{pmatrix} 1 & 2 \\ 2 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1x_1 + 2x_2 \\ 2x_1 + 0x_2 \\ 0x_1 + 1x_2 \end{pmatrix} = \begin{pmatrix} \text{inner products} \\ \text{of the rows} \\ \text{with } (x_1, x_2) \end{pmatrix}$$

→ This refers to the way of computing the matrix-vector product according to “**row · column**”.

We give this type of product of two vectors a special name:

Definition 1.10 (Inner product) Let $x, y \in \mathbb{F}^n$ be two vectors. Then the (standard) **inner product** of x and y is defined by

$$(x, y)_2 := \bar{x} \cdot y := \sum_{i=1}^n \bar{x}_i y_i = \bar{x}_1 y_1 + \cdots + \bar{x}_n y_n,$$

where \bar{x}_i denotes the complex conjugate.

- For real vectors $x, y \in \mathbb{R}^n$ this simplifies to

$$(x, y)_2 = \sum_{i=1}^n x_i y_i = x_1 y_1 + \cdots + x_n y_n.$$

- This operations is sometimes also called *scalar* or *dot product*. It is a central operation and we will illuminate some properties later on.

Example 1.11 (Inner products)

$$\begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} \cdot \begin{pmatrix} 3 \\ -1 \\ 1 \end{pmatrix} = 1 \cdot 3 + 2 \cdot (-1) + 0 \cdot 1 = 1, \quad \begin{pmatrix} 2+3i \\ i \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 1 \\ -i \\ 0 \end{pmatrix} = (\overline{2+3i}) \cdot 1 + \overline{i} \cdot (-i) + \overline{1} \cdot 0 = 2 - 3i + i^2 = 1 - 3i.$$

(2) By columns: Used for understanding

$$\begin{pmatrix} 1 & 2 \\ 2 & 0 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = x_1 \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} + x_2 \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} \text{linear combination} \\ \text{of the columns} \\ a_1, a_2 \end{pmatrix}$$

Definition 1.12 (Linear combination) Let $a_1, \dots, a_n \in \mathbb{F}^m$, $x \in \mathbb{F}^n$. Then

$$\sum_{i=1}^n x_i a_i = x_1 a_1 + \dots + x_n a_n = Ax \in \mathbb{F}^m$$

is called **linear combination** of the vectors a_1, \dots, a_n . Here, $A := [a_1, \dots, a_n] \in \mathbb{F}^{m \times n}$.

Example 1.13 (Linear combination)

Let us consider $\mathbb{F} = \mathbb{R}$ and again the vectors $a_1 := \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}$ and $a_2 = \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix}$.

Then examples of linear combinations are:

$$a_1 = 1 \cdot a_1 + 0 \cdot a_2,$$

$$a_2 = 0 \cdot a_1 + 1 \cdot a_2,$$

$$a_1 + a_2 = \dots,$$

....

[ex:picture]

The matrix product

We generalize the *matrix-vector* product above to a *matrix-matrix* product by observing that:

"A matrix is just a collection of columns (or vectors)."

Idea:

$$m \begin{pmatrix} \text{ } \\ \text{ } \\ \text{ } \\ \text{ } \\ \text{ } \end{pmatrix} \cdot r \begin{pmatrix} \text{ } \\ \text{ } \\ \text{ } \\ \text{ } \\ \text{ } \end{pmatrix} = m \begin{pmatrix} \text{ } \\ \text{ } \\ \text{ } \\ \text{ } \\ \text{ } \end{pmatrix}$$

$A \in \mathbb{F}^{m \times r}$ $B \in \mathbb{F}^{r \times n}$ $C \in \mathbb{F}^{m \times n}$

We make this a rigorous definition:

Definition 1.14 (Matrix-Matrix Product) For matrices $A \in \mathbb{F}^{m \times r}$ and $B \in \mathbb{F}^{r \times n}$, we define the **matrix-matrix product** (or simply **matrix product**) $C := A \cdot B \in \mathbb{F}^{m \times n}$ as a column wise product, i.e.,

$$\begin{pmatrix} c_{11} & c_{12} & \dots & c_{1n} \\ c_{21} & c_{22} & \dots & c_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ c_{m1} & c_{m2} & \dots & c_{mn} \end{pmatrix} = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1r} \\ a_{21} & a_{22} & \dots & a_{2r} \\ \vdots & \vdots & \ddots & \vdots \\ a_{m1} & a_{m2} & \dots & a_{mr} \end{pmatrix} \cdot \begin{pmatrix} b_{11} & b_{12} & \dots & b_{1n} \\ b_{21} & b_{22} & \dots & b_{2n} \\ \vdots & \vdots & \ddots & \vdots \\ b_{r1} & b_{r2} & \dots & b_{rn} \end{pmatrix}, \text{ i.e. } \boxed{\begin{aligned} c_{ij} &= \sum_{\ell=1}^r a_{i\ell} b_{\ell j} \\ i &= 1, \dots, m \\ j &= 1, \dots, n \end{aligned}}$$

Note that it is of utmost importance that the matrix dimensions fit in so far as the middle dimension of $A \in \mathbb{F}^{m \times r}$, $B \in \mathbb{F}^{r \times n}$ (i.e., r) is the same. Otherwise, this product cannot be formulated!

The (conjugate) Transpose Matrix

We finally introduce the operation of transposing matrices (and vectors):

Definition 1.16 (*Conjugate Transpose matrix*)

For a matrix $A := (a_{ij})_{ij} \in \mathbb{F}^{m \times n}$ the **conjugate (or Hermitian) transpose matrix** A^H of A is defined as

$$A^H := (\bar{a}_{ji})_{ij} \in \mathbb{F}^{n \times m},$$

where \bar{a}_{ji} denotes the complex conjugate of the coefficient a_{ji} .

For a real matrix $A := (a_{ij})_{ij} \in \mathbb{R}^{m \times n}$, so that $\bar{a}_{ji} = a_{ji}$, this simplifies to

$$A^\top := A^H = (a_{ji})_{ij} \in \mathbb{R}^{n \times m}$$

which we then simply call the **transpose matrix** A^\top of A .

Observe that we have the relation

$$A^H = \overline{A}^T,$$

where \overline{A} is understood as the component-wise complex conjugate.

Example 1.17 (*Conjugate transpose*)

- Transposing a matrix.
- Transposing a vector.
- The inner product can be written as $x^H y$ (or $x^\top y$ for real vectors).
- Adjoint operator: Consider a matrix $A = [a_1, a_2] \in \mathbb{R}^{3 \times 2}$ which maps $\mathbb{R}^2 \rightarrow \mathbb{R}^3$. Then $A^\top \in \mathbb{R}^{2 \times 3}$ maps $\mathbb{R}^3 \rightarrow \mathbb{R}^2$ and

$$A^\top p = \begin{pmatrix} a_1^\top p \\ a_2^\top p \end{pmatrix}$$

collects all inner products of p with the columns. We will relate the inner product to projections later on.

1.2 Span and Image – Linear Independence and Kernel

Example 1.19 (*Span and Image*)

Span: Let us again consider the two real vectors

$$a_1 = \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix}, \quad a_2 = \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix} \in \mathbb{R}^3.$$

Question: What are the vectors that we can represent as linear combination thereof?

There are two operations involved:

·: Scaling each vector a_1 and a_2 individually yields infinite lines through these vectors.

+: By adding arbitrary vectors from these lines we fill out the infinite plane in-between.

All combinations of these two vectors form an infinite plane in \mathbb{R}^3 . We say the plane is “spanned” by a_1 and a_2 .

The terminology for the set of all linear combinations is therefore accordingly:

$$\text{span}(a_1, a_2) := \left\{ x_1 \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} + x_2 \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix} : x_1, x_2 \in \mathbb{R} \right\}.$$

Image: By considering these two vectors as columns of a matrix, more precisely,

$$A = \begin{pmatrix} 1 & 2 \\ 2 & 0 \\ 0 & 1 \end{pmatrix},$$

the analogue notion is given by the so-called *image* of the matrix, which collects all matrix–vector products, i.e.,

$$\text{Im}(A) := \{Ax : x \in \mathbb{R}^2\} = \left\{ x_1 \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} + x_2 \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix} : x_1, x_2 \in \mathbb{R} \right\} = \text{span}(a_1, a_2).$$

The set of all possible linear combinations or matrix–vector products is given a special name:

Definition 1.20 (*Span and Image*)

i) *The span of vectors* $a_1, \dots, a_n \in \mathbb{F}^m$ is defined by

$$\text{span}(a_1, \dots, a_n) := \left\{ \sum_{i=1}^n x_i a_i : x_i \in \mathbb{F} \right\} \subset \mathbb{F}^m.$$

The set $\{a_1, \dots, a_n\}$ is called **generating system** of $\text{span}(a_1, \dots, a_n)$.

ii) *The image (or column space) of a matrix* $A := [a_1, \dots, a_n] \in \mathbb{F}^{m \times n}$ is defined by

$$\text{Im}(A) := \{Ax : x \in \mathbb{F}^n\} = \text{span}(a_1, \dots, a_n) \subset \mathbb{F}^m.$$

With this terminology we find

$$\text{"}Ax = b \text{ is solvable"} \Leftrightarrow b \text{ is spanned by the columns of } A \Leftrightarrow b \in \text{Im}(A).$$

[ex:picture]

Consider the example from above (i.e., $A := [a_1, a_2]$) and some vector $b = \begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix}$. By "solving" the system $Ax = b$ we want to find a linear combination of the columns a_1 and a_2 (i.e., scalars x_1 and x_2), so that this combination produces the vector b , i.e.,

$$Ax = b \Leftrightarrow x_1 \cdot | a_1 + x_2 \cdot | a_2 = b \Leftrightarrow x_1 \cdot \begin{pmatrix} 1 \\ 2 \\ 0 \end{pmatrix} + x_2 \cdot \begin{pmatrix} 2 \\ 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \\ 3 \end{pmatrix}.$$

In our example we find that this b is not contained in the span of the columns a_1, a_2 (= the infinite plane) so that our system is **not** solvable. In particular we find $\text{Im}(A) \subsetneq \mathbb{R}^3$ (we say f_A is not "surjective").

Let us properly define these concepts:

Definition 1.21 (*Linear independence and kernel*)

- i) Vectors $a_1, \dots, a_r \in \mathbb{F}^m$ are called **linearly independent**, if the only combination that gives the zero vector is $0a_1 + \dots + 0a_r$.
- ii) The **kernel** of a matrix $A \in \mathbb{F}^{m \times n}$ is defined by

$$\ker(A) := \{x \in \mathbb{F}^n : Ax = 0\},$$

i.e., the preimage of $\{0\}$ under f_A .

We find the following important equivalent formulation of linear independence:

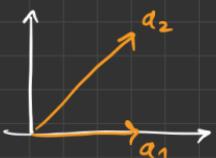
Lemma 1.22 For vectors $a_1, \dots, a_r \in \mathbb{F}^n$ we have the equivalence:

a_1, \dots, a_r linearly independent \Leftrightarrow every vector $b \in \text{span}(a_1, \dots, a_r)$ can be uniquely linearly combined from the set $\{a_1, \dots, a_r\}$, i.e.,
 $\exists_{1x_1, \dots, x_r \in \mathbb{F}}: b = x_1a_1 + \dots + x_ra_r.$

Remark. This result implies the following for solutions of linear systems: Let x solve $Ax = b$. If A has independent columns, then the solution x is unique! On the contrary, if the columns are dependent, we will learn that there are infinitely many solutions!

Summary: Relation between vector and matrix notions

$$a_1, \dots, a_n \in \mathbb{F}^m$$

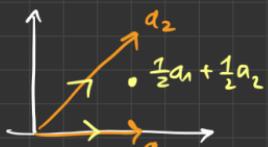


$$A = \begin{pmatrix} | & | \\ a_1 & \dots & a_n \\ | & | \end{pmatrix} \in \mathbb{F}^{m \times n}$$

LINEAR COMBINATION

$$\sum_{i=1}^n x_i a_i = x_1 a_1 + \dots + x_n a_n$$

$x_i \in \mathbb{F}$



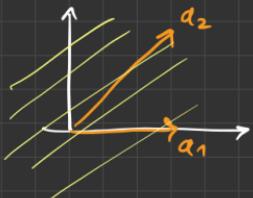
MATRIX-VECTOR PRODUCT

$$x = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix} \in \mathbb{F}^n$$

$$Ax = x_1 a_1 + \dots + x_n a_n$$

SPAN OF VECTORS

$$\text{span}(a_1, \dots, a_n) := \left\{ \sum_{i=1}^n x_i a_i : x_i \in \mathbb{F} \right\}$$



IMAGE

$$\text{Im } A := \{Ax : x \in \mathbb{F}^n\}$$

LINEARLY INDEPENDENT

a_1, \dots, a_n are called independent



$$Ax = x_1 a_1 + \dots + x_n a_n = 0 \quad \Rightarrow \quad \Leftrightarrow \quad x_i = 0$$

$\Leftarrow \checkmark$



KERNEL

$$\ker A := \{x \in \mathbb{F}^n : Ax = 0\}$$

1.3 Subspaces of \mathbb{F}^n – Basis and Dimension

Example 1.23 (*Subspaces*)

Let $\mathbb{F} = \mathbb{R}$.

- $n = 2$: A straight line $L := \{xa : x \in \mathbb{R}\} \subset \mathbb{R}^2$ spanned by a fixed $a \in \mathbb{R}^2$. For a linear function $f(x) = mx$ with $m := \frac{a_2}{a_1}$ we find

$$\text{graph}(f) := \{(x, f(x)) : x \in \mathbb{R}\} = \{(x, mx) : x \in \mathbb{R}\} = \text{span}\left(\begin{pmatrix} 1 \\ \frac{a_2}{a_1} \end{pmatrix}\right) = \text{span}\left(\begin{pmatrix} a_1 \\ a_2 \end{pmatrix}\right) \quad (\text{note: } a_1\mathbb{R} = \mathbb{R})$$

- $n = 3$: A plane $P := \{x_1a_1 + x_2a_2 : x_i \in \mathbb{R}\} \subset \mathbb{R}^3$ spanned by fixed $a_1, a_2 \in \mathbb{R}^3$.
- Not a (linear) subspace: The graph of nonlinear functions, such as x^2 or $\sin(x)$ in \mathbb{R}^2 .

[ex:pictures]

Definition 1.24 (*Subspace*) A subset $V \subset \mathbb{F}^n$ is called **(linear) subspace of \mathbb{F}^n** if

- i) it is nonempty, i.e., $V \neq \emptyset$,
- ii) and if it is closed under linear combinations, i.e., if

$$\lambda_1v_1 + \lambda_2v_2 \in V \quad \text{for all } v_1, v_2 \in V, \lambda_1, \lambda_2 \in \mathbb{F}.$$

Question: Is it possible to describe a linear subspace of \mathbb{F}^n by a finite number of vectors?

Definition 1.25 (Basis) Let $V \subset \mathbb{F}^n$ be a subspace of \mathbb{F}^n . Then a set of vectors $\{v_1, \dots, v_r\} \subset V$ with $r \leq n$ is called **basis** of V , if

- i) v_1, \dots, v_r are linearly independent,
- ii) $\text{span}(v_1, \dots, v_r) = V$.

- Let $\{v_1, \dots, v_r\} \subset V$ be a basis. Then, in particular, any $v \in V = \text{span}(v_1, \dots, v_r)$ can be written as

$$v = \sum_{j=1}^r \lambda_j v_j$$

for some uniquely determined scalars $\lambda_j \in \mathbb{F}$ (see Lemma ??).

→ These scalars are called **coordinates** of v with respect to the basis $\{v_1, \dots, v_r\}$.

- One can show that
 - there exists a basis (general result based on Zorn's lemma),
 - any basis of a subspace of \mathbb{F}^n has the same length (doable proof), which we call **dimension of V** ($\dim(V)$).
- With other words:

The maximum number of linearly independent vectors is called dimension and the set of such vectors is called a basis.

Example 1.26

1) Let us consider $\mathbb{F} = \mathbb{R}$ and $V := \mathbb{R}^2 \subset \mathbb{R}^2$.

We first show that V is a subspace of \mathbb{R}^2 and then try to find some bases.

Following Definition ?? we show:

- i) $V \neq \emptyset$: Consider $0 \in V$.
- ii) V is closed under linear combinations: Let $v_1, v_2 \in V$, $\lambda_1, \lambda_2 \in \mathbb{R}$, then clearly $\lambda_1 v_1 + \lambda_2 v_2 \in \mathbb{R}^2 = V$.

Now it makes sense to talk about a *basis* for V . We next try to find a set of vectors $v_1, \dots, v_r \in V$ that satisfies Definition ??.

1a) Let us consider the vectors $e_j := (\delta_{ij})_{1 \leq i \leq n} = (0 \dots 1 \dots 0)^\top \in \mathbb{R}^n$, here with $n = 2$. We show that $\{e_1, e_2\}$ is a basis of V by verifying the two conditions in Definition ??.

- i) We show that e_1, e_2 are linearly independent. From

$$x_1 e_1 + x_2 e_2 = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} \stackrel{!}{=} 0$$

we easily conclude that $x_1 = 0 = x_2$, so that e_1, e_2 are indeed linearly independent.

- ii) By Definition ?? any $v = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix} \in V = \mathbb{R}^2$ can be written as

$$v = v_1 \begin{pmatrix} 1 \\ 0 \end{pmatrix} + v_2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = v_1 e_1 + v_2 e_2.$$

Thus

$$V = \mathbb{R}^2 = \{v_1 e_1 + v_2 e_2 : v_1, v_2 \in \mathbb{R}\} = \text{span}(e_1, e_2).$$

In terms of the previous slide, we have that v_1, v_2 are the coordinates of v w.r.t the basis $\{e_1, e_2\}$ and the dimension of V is 2, we write $\dim(V) = 2$.

Remark: Analogue results hold true for any \mathbb{R}^n (not just $n = 2$) and the set of vectors $\{e_1, \dots, e_n\}$ is called the standard basis or unit vectors in \mathbb{R}^n .

- 1b) Let us find another basis for \mathbb{R}^2 and check whether its length is still 2 in accordance with the remarks after Definition ??.
- For instance, let us consider the vectors

$$a_1 = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, \quad a_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix} \in V.$$

Again, we verify that the two conditions in Definition ?? are satisfied:

- i) Now let us use the equivalent formulation of linear independence from Lemma ???. For this purpose let $v \in \text{span}(a_1, a_2)$ so that there exist scalars $\lambda_1, \lambda_2 \in \mathbb{R}$ with

$$\begin{pmatrix} v_1 \\ v_2 \end{pmatrix} = \lambda_1 a_1 + \lambda_2 a_2,$$

which, after inserting the precise numbers for a_1 and a_2 , is equivalent to

$$\begin{pmatrix} \lambda_1 \\ 0 \end{pmatrix} + \begin{pmatrix} \lambda_2 \\ \lambda_2 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}.$$

Using matrix notation we can even write

$$\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \cdot \begin{pmatrix} \lambda_1 \\ \lambda_2 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}.$$

In order to apply Lemma ??, we need to show that the scalars λ_1, λ_2 are uniquely determined by this equation. Therefore, let us now solve this upper triangular system (we will later learn about *backward substitution* to do this algorithmically). We observe from the bottom equation that $\lambda_2 = v_2$. Inserting this into the top equation then yields

$$\lambda_1 + \lambda_2 = v_1 \Leftrightarrow \lambda_1 + v_2 = v_1 \Leftrightarrow \lambda_1 = v_1 - v_2.$$

Observe that λ_1 and λ_2 are uniquely determined, i.e., there are no other λ_1 and λ_2 solving the upper equations; thus a_1, a_2 are independent by Lemma ???. Also, let us make a quick test:

$$(v_1 - v_2)a_1 + v_2a_2 = \begin{pmatrix} v_1 - v_2 \\ 0 \end{pmatrix} + \begin{pmatrix} v_2 \\ v_2 \end{pmatrix} = \begin{pmatrix} v_1 \\ v_2 \end{pmatrix}.$$

- ii) We note that $\text{span}(a_1, a_2) \subset \mathbb{R}^2 = V$ is obviously true and to prove the reverse subset relation we choose the scalars $\lambda_1 = v_1 - v_2$, $\lambda_2 = v_2$ for $v = (v_1, v_2)^\top \in V = \mathbb{R}^2$.

All in all, we have that $\lambda_1 = v_1 - v_2$, $\lambda_2 = v_2$ are the coordinates of $v \in V$ w.r.t the basis $\{a_1, a_2\}$ of V and $\dim(V) = 2$.

Remark: The notation for vectors introduced in D. ?? implicitly assumes that vectors are represented in the standard basis.

In the exercises we will prove that for any matrix $A \in \mathbb{F}^{m \times n}$, the kernel $\ker(A)$ is a subspace of \mathbb{F}^n and the image $\text{Im}(A)$ is a subspace of \mathbb{F}^m . In the context of matrices these are important spaces and we give their dimensions a special name:

Definition 1.27 (rank and nullity) Let $A \in \mathbb{F}^{m \times n}$. Then

- $\text{rank}(A) := \dim(\text{Im}(A))$ is called the (column) **rank of A** ,
- $\text{nullity}(A) := \dim(\ker(A))$ is called the **nullity of A** .

Example 1.28

1) Let us consider the matrix $A = [a_1, a_2, a_3] := \begin{pmatrix} 1 & 1 & 2 \\ 0 & 1 & 1 \end{pmatrix}$.

1a) By Definition ?? of the image we have $\text{Im}(A) = \text{span}(a_1, a_2, a_3)$. By observing $a_3 = a_2 + a_1$, i.e., a_3 is a linear combination of a_1 and a_2 , we even find that $\text{Im}(A) = \text{span}(a_1, a_2)$. Since the vectors a_1, a_2 have been identified to be linearly independent (see Example ??), we find by Definition ?? that they form a basis for $\text{Im}(A)$. Thus

$$\text{rank}(A) = \dim(\text{Im}(A)) = 2.$$

1b) What about the nullity? We first need to find a basis of the kernel (we will do this by re-writing it as a span of some independent vectors). For this purpose, let $x \in \ker(A)$, which by Definition ?? is equivalent to

$$Ax = 0 \Leftrightarrow x_1 + x_2 + 2x_3 = 0, \quad x_2 + x_3 = 0.$$

Now from the second equation we obtain $x_2 = -x_3$. Let us also write x_1 as a function of x_3 . This is achieved by inserting $x_2 = -x_3$ into the first equation to obtain

$$x_1 + x_2 + 2x_3 = x_1 - x_3 + 2x_3 = x_1 + x_3 = 0 \Leftrightarrow x_1 = -x_3.$$

Thus we find

$$Ax = 0 \Leftrightarrow x = \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} = \begin{pmatrix} -x_3 \\ -x_3 \\ x_3 \end{pmatrix} = x_3 \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}.$$

With other words, we can write

$$\ker(A) = \left\{ \begin{pmatrix} x_1 \\ x_2 \\ x_3 \end{pmatrix} \in \mathbb{R}^3 : x = x_3 \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} \right\} = \left\{ x_3 \cdot \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} : x_3 \in \mathbb{R} \right\} = \text{span}\left(\begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}\right).$$

Since $\begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} \neq 0$ it forms an independent set of length 1 so that by Definitions ?? and ?? we finally conclude that

$$\text{nullity}(A) = \dim(\ker(A)) = 1.$$

Remark: We observe that

$$\text{rank}(A) + \text{nullity}(A) = 3 \quad (= \text{column dimension}).$$

We will see below that this is generally true – called the dimension formula!

2) Let us consider $A = [a_1, a_2] := \begin{pmatrix} 1 & 2 \\ 1 & 2 \\ 0 & 0 \end{pmatrix}$.

2a) Since $a_2 = 2 \cdot a_1$, the columns are certainly linearly dependent (e.g., $2 \cdot a_1 + (-1)a_2 = 0 \in \mathbb{R}^2$; a combination that yields zero but with nonzero coefficients). Therefore

$$\text{Im}(A) = \text{span}(a_1, a_2) = \text{span}(a_1),$$

so that

$$\text{rank}(A) = \dim(\text{Im}(A)) = 1.$$

2b) Now let us consider the kernel $\ker(A) = \{x : Ax = 0\}$. Following along the lines of the previous slides we get

$$Ax = 0 \Leftrightarrow \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} x_1 + \begin{pmatrix} 2 \\ 2 \\ 0 \end{pmatrix} x_2 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Leftrightarrow \begin{pmatrix} x_1 + 2x_2 \\ x_1 + 2x_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} \Leftrightarrow x_1 = -2x_2$$

and thus

$$\ker(A) = \{x \in \mathbb{R}^2 : x_1 = -2x_2\} = \left\{ \begin{pmatrix} -2x_2 \\ x_2 \end{pmatrix} \in \mathbb{R}^2 : x_2 \in \mathbb{R} \right\} = \{x_2 \begin{pmatrix} -2 \\ 1 \end{pmatrix} \in \mathbb{R}^2 : \lambda \in \mathbb{R}\} = \text{span} \left(\begin{pmatrix} -2 \\ 1 \end{pmatrix} \right).$$

So all in all, $\text{nullity}(A) = \dim(\ker(A)) = 1$.

Remark: Again we observe that

$$\text{rank}(A) + \text{nullity}(A) = 2 \quad (= \text{column dimension}).$$

3) Similarly, considering the matrices from above we find $\text{rank}(A_2) = 2$ and $\text{rank}(A_3) = 3$.

Question: Can we find a general relation between the nullity and the rank of a matrix?

Theorem 1.29 (Dimension Formula/Rank–Nullity Theorem) Let $A \in \mathbb{F}^{m \times n}$, then

$$\text{rank}(A) + \text{nullity}(A) = n.$$

- The dimension formula also reads as

$$\dim(\text{Im}(A)) + \dim(\ker(A)) = \dim(\mathbb{F}^n).$$

- **Intuition:** Let us again think of a matrix $A \in \mathbb{F}^{m \times n}$ as a mapping from \mathbb{F}^n to \mathbb{F}^m . If the matrix maps some vectors of this n -dimensional space \mathbb{F}^n to 0 – precisely those vectors from the kernel of A – then we can say that this “piece of information” gets lost. What prevails from \mathbb{F}^n makes up the image of A whose dimension is the rank of the matrix by definition. So, the amount of information in \mathbb{F}^n equals the information that gets lost after mapping it by A ($\text{nullity}(A)$) plus the one that prevails ($\text{rank}(A)$).

1.4 Inverse Matrices

Example 1.30 (Inverses) Let us consider the following matrix

$$A = [a_1, a_2] = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix},$$

which is composed of the vectors considered in Example ?? 1b).

Recall results Ex.?? 1b): We have already observed that a_1, a_2 are independent and $\text{span}(a_1, a_2) = \mathbb{R}^2$. With other words, for any $b \in \mathbb{R}^2$, by Lemma ?? there exist unique (!) scalars x_1, x_2 , so that $Ax = x_1 a_1 + x_2 a_2 = b$.

More precisely, for $x_b = \begin{pmatrix} b_1 - b_2 \\ b_2 \end{pmatrix}$ (coordinates of b wrt. the basis $\{a_1, a_2\}$) we found

$$Ax_b = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} b_1 - b_2 \\ b_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix} = b.$$

Clearly, the vector x_b is composed of information from b . Now let us consider the following mapping

$$b \mapsto x_b = \begin{pmatrix} b_1 - b_2 \\ b_2 \end{pmatrix} = \underbrace{\begin{pmatrix} 1 \\ 0 \end{pmatrix} b_1 + \begin{pmatrix} -1 \\ 1 \end{pmatrix} b_2}_{=: A^{-1}} = \underbrace{\begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix}}_{=: A^{-1}} \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}.$$

We observe that the mapping from the vector b to its coordinates x_b w.r.t. the basis $\{a_1, a_2\}$ can be expressed as a matrix–vector product. The involved matrix A^{-1} is referred to as the *inverse matrix* of A .

In general:

Consider the matrix as a mapping

$$f_A : \mathbb{F}^n \rightarrow \mathbb{F}^n, x \mapsto Ax.$$

Then by definition the *mapping* f_A is **invertible**, if there exists a mapping $f_A^{-1} : \mathbb{F}^n \rightarrow \mathbb{F}^n$ such that for all $x, b \in \mathbb{F}^n$ we have

$$f_A(x) = b \Leftrightarrow x = f_A^{-1}(b).$$

Inserting the definition of f_A this reads as

$$Ax = b \Leftrightarrow x = A^{-1}b.$$

Verifying this condition for all possible x and b would be an ambitious endeavor. Luckily, this condition can be rephrased into conditions solely involving the matrix A . More precisely, by inserting one into the other we obtain

- i) $Ax = b \Leftrightarrow AA^{-1}b = b \Leftrightarrow AA^{-1} = I,$
- ii) $x = A^{-1}b \Leftrightarrow x = A^{-1}Ax \Leftrightarrow A^{-1}A = I.$

Let us quickly check this for Example ??:

$$A^{-1}A = \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I_2 \quad \checkmark, \quad AA^{-1} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & -1 \\ 0 & 1 \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} = I_2 \quad \checkmark.$$

Let us make this a definition.

Definition 1.31 (Inverse matrix) A matrix $A \in \mathbb{F}^{n \times n}$ is called **invertible**, if there exists a matrix $\tilde{A} \in \mathbb{F}^{n \times n}$ with

$$A \cdot \tilde{A} = \tilde{A} \cdot A = I_n. \quad (5)$$

In case of existence we find that \tilde{A} is unique (see below) and we denote by $A^{-1} := \tilde{A}$ the **inverse matrix** of A . The set of all invertible matrices in $\mathbb{F}^{n \times n}$ is denoted by $GL_n(\mathbb{F})$, the so-called general linear group.

Consider the linear equation

$$Ax = b$$

By setting $x := A^{-1}b$, we find

$$Ax = AA^{-1}b = AA^{-1}b = I_n b = b.$$

If A is invertible, then

"solving $Ax = b$ " = "applying the inverse matrix A^{-1} "

(numerical methods) (not accessible in practice)

From the dimension formula ?? for $n = m$, we find "injectivity = surjectivity"

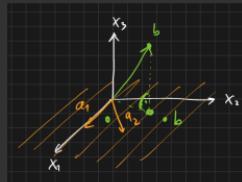
$$A = \begin{pmatrix} 1 & & \\ a_1 - a_n & \ddots & \\ 1 & & 1 \end{pmatrix} \in \mathbb{F}^{n \times n}, \quad f_A : \mathbb{F}^n \rightarrow \mathbb{F}^n, \quad x \mapsto Ax$$

mapping f_A	matrix A	vectors (columns) a_1, \dots, a_n
f_A injective	\Leftrightarrow Ex. $\ker A = \{0\}$	a_1, \dots, a_n are independent
	\Leftrightarrow $\dim(\ker A) = 0$	
	\Leftrightarrow [DIMENSION FORMULA]	\Leftrightarrow
	$\dim(\text{Im } A) = n - \dim(\ker A) = n$	
f_A surjective	\Leftrightarrow $\underbrace{\text{Im } A = \mathbb{F}^n}_{f_A(\mathbb{F}^n)}$	$\text{span}(a_1, \dots, a_n) = \mathbb{F}^n$

Also see Lemma ??

Remark:

A System $Ax = b$ can be solvable even if A is not squared (and thus not invertible)!



The Difference:

- *invertible* ($m = n$): For **any** b there is a **unique** x so that $Ax = b$, i.e.,

$$A \text{ is invertible} \Rightarrow \text{we always have that } b \in \text{Im}(A)$$

This unique x is given by $A^{-1}b$.

- *solvable* ($m \neq n$ allowable): Given a **fixed** b we find **at least one** x so that $Ax = b$, i.e.,

$$Ax = b \text{ is solvable} \Leftrightarrow b \in \text{Im}(A)$$

We will learn later that in some cases this x is given by $(A^\top A)^{-1}A^\top b$.

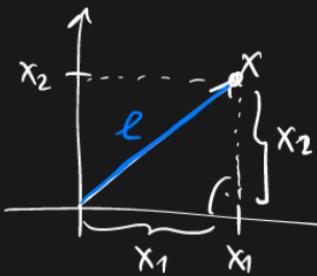
Thus:

$$\text{invertible} \Rightarrow \text{solvable}$$

1.5 The Euclidean Norm

Let us first consider the 2d and 3d case:

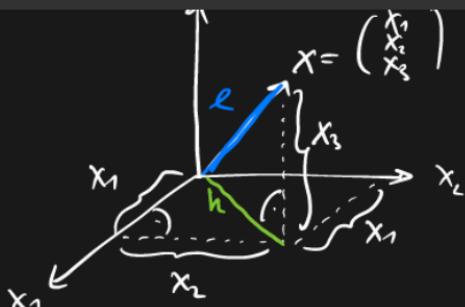
2d:



$$\begin{aligned} e^2 &= x_1^2 + x_2^2 \\ \Leftrightarrow e &= \sqrt{x_1^2 + x_2^2} \\ &= \sqrt{(x, x)_2} \end{aligned}$$

$$(x, y)_2 := \sum_{i=1}^n x_i y_i$$

3d:



$$\begin{aligned} e^2 &= h^2 + x_3^2 = x_1^2 + x_2^2 + x_3^2 \\ \Leftrightarrow e &= \sqrt{x_1^2 + x_2^2 + x_3^2} = \sqrt{(x, x)_2} \\ \sqrt{(x, x)_2} &= \sqrt{\sum_{i=1}^n x_i \cdot x_i} = \sqrt{\sum_{i=1}^n x_i^2} = \sqrt{x_1^2 + x_2^2 + x_3^2} \end{aligned}$$

This idea can be generalized to:

Definition 1.33 (Euclidean Norm) The Euclidean norm of a vector $x \in \mathbb{F}^n$ is defined by

$$\|x\|_2 := \sqrt{\sum_{i=1}^n |x_i|^2} = \sqrt{x^H x}$$

where $|a + ib|^2 := a^2 + b^2$ denotes the absolute value of a complex number. For a real vector $x \in \mathbb{R}^n$ this simplifies to $\|x\|_2 := \sqrt{\sum_{i=1}^n x_i^2} = \sqrt{x^\top x}$.

→ We will also get to know other “norms” (e.g., Manhattan norm or maximum norm).

Relating the inner product to projections

Let us consider $\mathbb{F} = \mathbb{R}$. As a special case of the so-called **Cauchy Schwarz inequality** one can show that, for any two real vectors $x, y \in \mathbb{R}^n$,

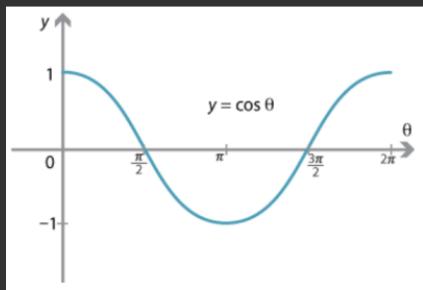
$$|x^T y| \leq \|x\|_2 \cdot \|y\|_2.$$

This is equivalent to (assumed both vectors are nonzero, otherwise trivial case)

$$-1 \leq \frac{x^T y}{\|x\|_2 \cdot \|y\|_2} = \left(\frac{x}{\|x\|_2} \right)^T \left(\frac{y}{\|y\|_2} \right) \leq 1.$$

Since $\cos: (0, \pi) \rightarrow (-1, 1)$ is bijective, we find an uniquely defined angle $\alpha \in (0, \pi)$, so that

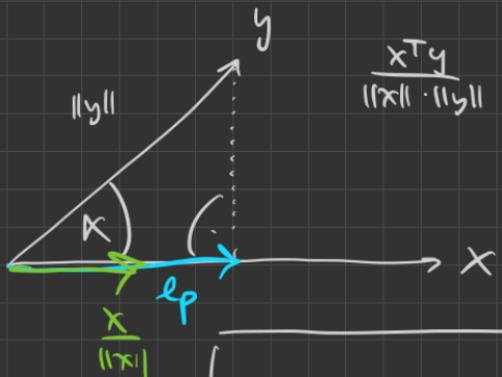
$$\cos(\alpha) = \frac{x^T y}{\|x\|_2 \cdot \|y\|_2} \quad (\in (-1, 1)).$$



We also use the notation $\alpha := \sphericalangle(x, y)$, since α can be considered 'the angle between x and y '.

Geometric insights from the identity

$$\text{cosine} = \frac{\text{adjacent}}{\text{hypotenuse}}.$$



$$\frac{x^T y}{\|x\| \cdot \|y\|} = \cos(\alpha) = \frac{e_p}{\|y\|} \iff$$

$$e_p = \frac{x^T y}{\|x\|}$$

$$\boxed{\text{proj}_x(y) = \frac{x}{\|x\|} \cdot e_p = \left(\frac{x^T y}{\|x\|} \right) \cdot \frac{x}{\|x\|}}$$



1.6 Orthogonal Vectors and Matrices

Let us again consider the relation

$$\cos(\alpha) = \frac{x^T y}{\|x\|_2 \cdot \|y\|_2}, \quad x, y \in \mathbb{R}^n.$$

Now let us assume that the angle $\alpha = \angle(x, y)$ between the two vectors x, y is 90° , i.e., $\alpha = \pm \frac{\pi}{2}$, meaning that they are *perpendicular*. Then we find

$$0 = \cos\left(\pm \frac{\pi}{2}\right) = \frac{x^T y}{\|x\|_2 \cdot \|y\|_2} \quad \Leftrightarrow \quad 0 = x^T y.$$

In mathematics we call this *orthogonal* and make it a general definition:

Definition 1.34 (Orthogonal/-normal vectors)

- i) Two vectors $x, y \in \mathbb{F}^n$ are called **orthogonal** if $(x, y)_2 = x^H y = 0$.
- ii) Two vectors $x, y \in \mathbb{F}^n$ are called **orthonormal** if they are orthogonal and have length 1 (i.e., $\|x\|_2 = \|y\|_2 = 1$).
- iii) Vectors $x_1, \dots, x_r \in \mathbb{F}^n$ are called (mutually) **orthogonal (orthonormal)** if x_i, x_j are orthogonal (orthonormal) for all possible pairs $i \neq j \in \{1, \dots, r\}$.

One can show that:

$$x, y \text{ orthogonal} \Rightarrow x, y \text{ linearly independent.} \tag{6}$$

Counter example for backwards implication: $x = \begin{pmatrix} 1 \\ 0 \end{pmatrix}, y = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

Example 1.35

For $\mathbb{F} = \mathbb{R}$ and $n = 2$ consider, e.g.,

- Standard basis vectors.
- Rotation of the standard basis vectors.

Now let us extend this notion to matrices:

For this purpose observe that the matrix-matrix product $Q^H Q$ for $Q \in \mathbb{F}^{n \times n}$ contains all possible inner products of its columns:

$$\underbrace{\begin{pmatrix} - & \bar{q}_1^\top & - \\ - & \bar{q}_2^\top & - \\ \vdots & & \\ - & \bar{q}_n^\top & - \end{pmatrix}}_{Q^H} \underbrace{\begin{pmatrix} | & | & & | \\ q_1 & q_2 & \cdots & q_n \\ | & | & & | \end{pmatrix}}_Q = \begin{pmatrix} q_1^H q_1 & \cdots & q_1^H q_n \\ q_2^H q_1 & \cdots & q_2^H q_n \\ \vdots & \ddots & \vdots \\ q_n^H q_1 & \cdots & q_n^H q_n \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}$$

Let us assume that the columns of Q are mutually orthonormal, then

$$Q^H Q = I_n.$$

Since this is a central property, we make this a definition:

Definition 1.36 (Orthogonal/Unitary matrix) A matrix $Q \in \mathbb{F}^{n \times n}$ is called **unitary**, if

$$Q^H Q = I_n.$$

For a real matrix $Q \in \mathbb{R}^{n \times n}$ this condition simplifies to $Q^T Q = I_n$, in which case we then call the matrix **orthogonal**.

Since orthogonality implies linear independence (see statement (??)) we know that **orthogonal matrices are invertible**. From the defining equation $Q^T Q = I_n$ we can even deduce its inverse

$$Q^{-1} = Q^T$$

and therefore also $QQ^T = I_n$.

→ This is one (of the many) reasons why the property of orthogonality is very desirable.

Understanding $QQ^\top(\cdot)$ as orthogonal projection

For a vector $q \in \mathbb{R}^n$ of length 1, i.e., $\|q\|_2 = 1$, and a vector $y \in \mathbb{R}^n$ we find

$$\text{proj}_q(y) = (q^\top y) \cdot q.$$

Now let $Q = [q_1, \dots, q_n] \in \mathbb{R}^{n \times n}$ be an orthogonal matrix (i.e., columns q_i are mutually orthonormal), then

$$y = I \cdot y = QQ^\top y = Q \begin{pmatrix} q_1^\top y \\ \vdots \\ q_n^\top y \end{pmatrix} = \sum_{i=1}^n q_i^\top y \cdot q_i = \sum_{i=1}^n \text{proj}_{q_i}(y).$$

In other words, in order to obtain the coordinates of y with respect to the *orthonormal* basis $\{q_1, \dots, q_n\}$ we solely have to project y onto each basis vector q_i .

Example

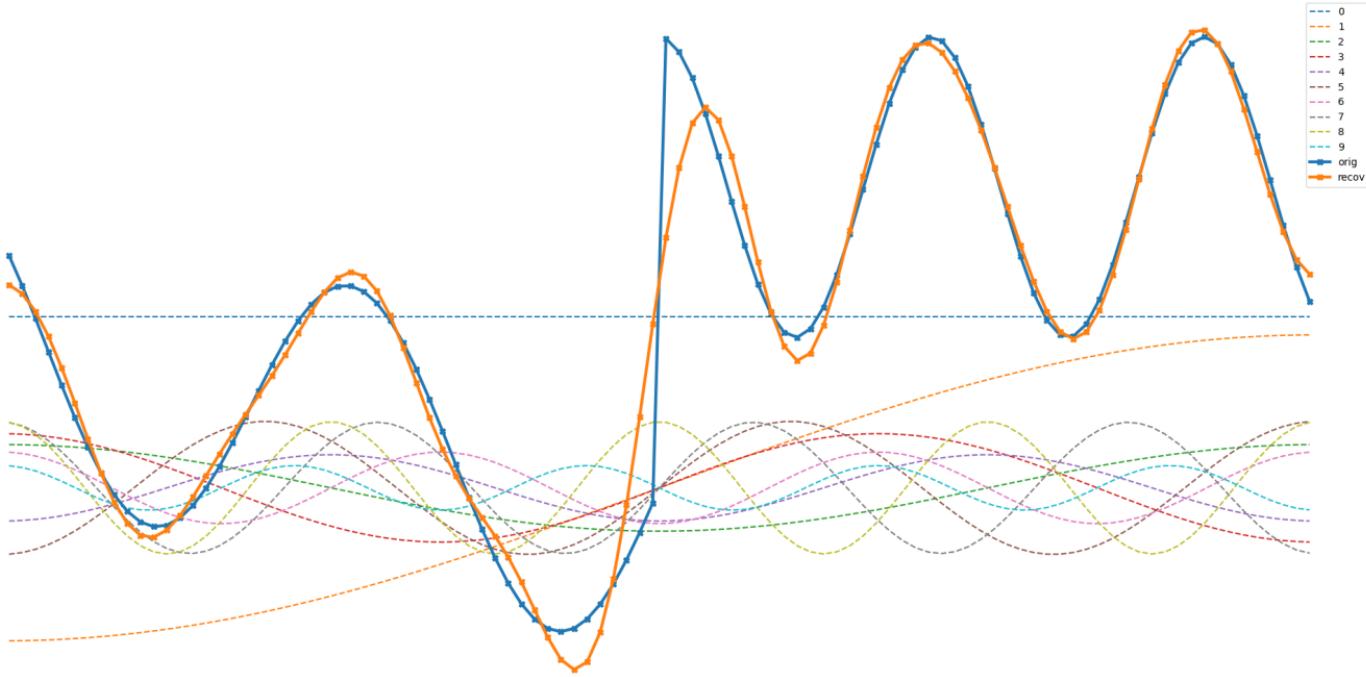
Famous related examples from signal processing include the Discrete Cosine Transform (DCT) and the Discrete Fourier Transform (DFT) which can be written as a matrix–vector product $Q^\top(\cdot)$ with an orthogonal/unitary matrix Q . In this context, the q_i may correspond to discrete periodic functions of different frequency. For a time-discrete signal

$$y = (y_1, \dots, y_n)^\top \in \mathbb{R}^n$$

one says that the transformed signal

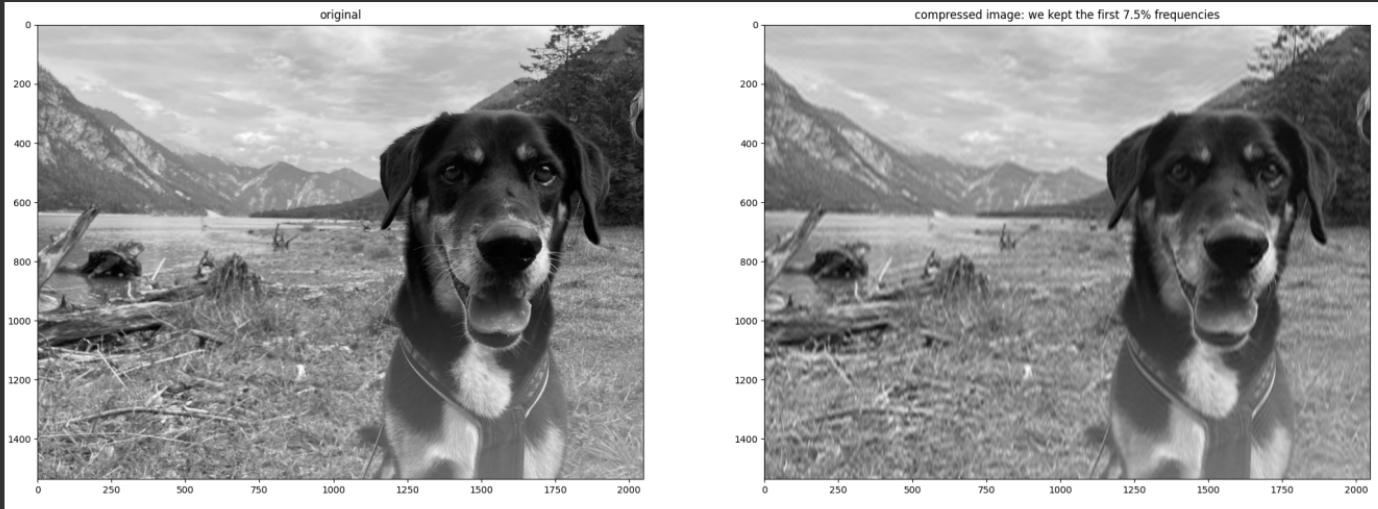
$$Q^\top y = (q_1^\top y, \dots, q_n^\top y)^\top$$

lives in the frequency space.



1-d DCT compression example (where high frequencies are removed):

$$y = \sum_{i=1}^n q_i^\top y \cdot q_i \approx \sum_{i=1}^m q_i^\top y \cdot q_i \quad (m < n).$$



2-d DCT compression example (where high frequencies are removed)

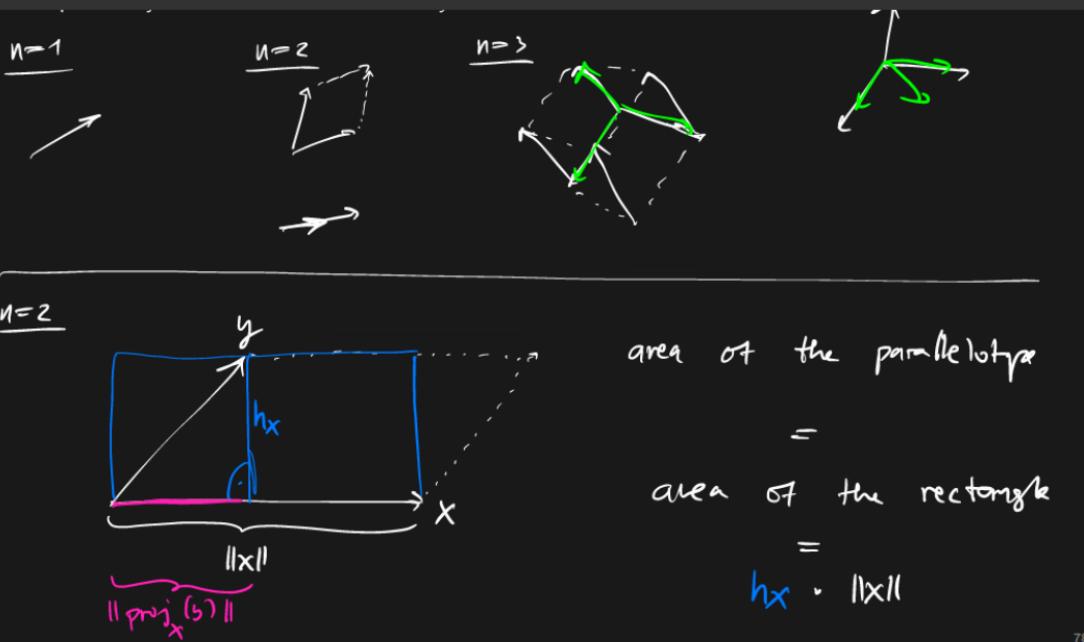
1.7 The Determinant

Aim: For n vectors in \mathbb{F}^n we want to have a *measure of linear independence*

- or equivalently a *volume measure* for the parallelotope spanned by these vectors
- or equivalently a *measure for the invertibility* of a matrix in $\mathbb{F}^{n \times n}$

Why are all these measures the same?

- n linear dependent vectors do not span a volume in \mathbb{F}^n .
- Linear independent columns of a quadratic matrix imply invertibility.



In general, there is the following (recursive) formula, which we use as the definition here:

Definition 1.37 (Laplace formula) Let $A \in \mathbb{F}^{n \times n}$ and let $A_{ij} \in \mathbb{F}^{(n-1) \times (n-1)}$ be the matrix resulting from erasing the i -th row and j -th column. Then the mapping $\det: \mathbb{F}^{n \times n} \rightarrow \mathbb{F}$ defined by

$$\det(A) = \sum_{j=1}^n (-1)^{i+j} a_{ij} \det(A_{ij}), \quad \text{for a fixed but arbitrary } i \in \{1, \dots, n\},$$

is called the **determinant** (of A), where $\det(a) := a$ for $a \in \mathbb{R} = \mathbb{R}^{1 \times 1}$.

One can show: The determinant is a well-defined function, i.e., by the formula above the function $\det(\cdot)$ assigns to each matrix $A \in \mathbb{F}^{n \times n}$ exactly one number in \mathbb{F} .

Laplace formula for $n = 2$ and $n = 3$:

- $n = 2$ (we fix $i = 1$)

Here we have

$$\det(A) = \sum_{j=1}^2 (-1)^{1+j} a_{1j} \det(A_{1j})$$

$$A_{11} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = [a_{22}], \quad A_{12} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = [a_{21}], \quad A_{21} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = [a_{12}], \quad A_{22} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix} = [a_{11}]$$

So that all in all

$$\det(A) = (-1)^{1+1} a_{11} \det(A_{11}) + (-1)^{1+2} a_{12} \det(A_{12}) = a_{11} \cdot a_{22} - a_{12} \cdot a_{21}$$

- $n = 3$: *Sarrus rule* (exercise)

One can show:

Theorem 1.38 (Determinant properties) *The determinant satisfies the following computational rules:*

- i) $\forall A \in \mathbb{F}^{n \times n} : \det(A) \neq 0 \Leftrightarrow A \in GL(n, \mathbb{F})$ (\Leftrightarrow columns of A are linearly independent)
- ii) $\forall A \in \mathbb{F}^{n \times n} : \det(A^\top) = \det(A)$
- iii) if $A \in \mathbb{F}^{m \times m}, B \in \mathbb{F}^{m \times n}, C \in \mathbb{F}^{n \times n}$ and

$$M := \begin{pmatrix} A & B \\ 0 & C \end{pmatrix} \in \mathbb{F}^{(m+n) \times (m+n)}$$

then $\det M = \det A \cdot \det C$

- iv) $\forall A, A' \in \mathbb{F}^{n \times n} : \det(A \cdot A') = \det(A) \cdot \det(A')$

The central result for us is i).

Question: Are there matrices for which the computation of the determinant is easy?

Yes, as in many other situations it turns out that orthogonal and triangular matrices are easy to treat! More precisely, we find:

Corollary 1.39 (Triangular matrices) Let $U \in \mathbb{F}^{n \times n}$ be upper triangular, i.e.,

$$U = \begin{pmatrix} u_{11} & x & \cdots & x \\ 0 & u_{22} & & \vdots \\ \vdots & & \ddots & x \\ 0 & \cdots & 0 & u_{nn} \end{pmatrix}.$$

Then

$$\det(U) = u_{11} \cdot u_{22} \cdot \dots \cdot u_{nn}.$$

In particular, we find

$$U \text{ is invertible} \Leftrightarrow \det(U) \neq 0 \Leftrightarrow \forall i : u_{ii} \neq 0$$

Proof. Exercise: For the product formula apply Theorem ?? iii) inductively. The second part then easily follows from Theorem ?? i). □

Corollary 1.40 (Orthogonal matrices) Let $Q \in \mathbb{R}^{n \times n}$ be an orthogonal matrix, then $|\det(Q)| = 1$.

Proof. From Cor. ?? we find $\det(I) = 1$. Then result follows from Theorem ?? ii) and iv). □

1.8 Linear Systems of Equations

Aim:

Given $A \in \mathbb{R}^{m \times n}$ ($m \neq n$ possible) and $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ such that
 $Ax = b$.

1.8.1 Motivation: Curve Fitting

As a motivating example let us consider *curve fitting*.

Assume we are given $m \in \mathbb{N}$ measurements $(z_1, y_1), \dots, (z_m, y_m) \in \mathbb{R}^2$ (or more generally in any product space, say $Z \times Y$)



Question: Is there a “significant” relation between the z_i and y_i ?

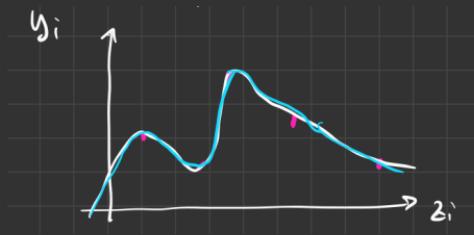
Let us consider the z_i as input (independent/explanatory/exogenous) variable, and the y_i as output (dependent/predicted/response...) variable.

Examples: $z_i = (\text{temperature, light intensity})$, $y_i = \text{plant height}$ or $z_i = \text{year}$, $y_i = \text{global mean temperature}$

Mathematically asking: Is there a function f , so that $f(z_i) \cong y_i$ for all $i = 1, \dots, m$?

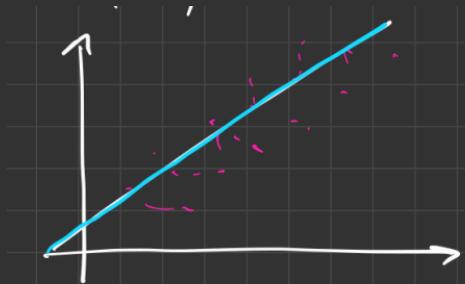
Exact fit: Interpolation

$$f(z_i) = y_i \quad \forall i = 1, \dots, m$$



Approximate fit: Regression/Smoothing

$$f(z_i) \approx y_i \quad \forall i = 1, \dots, m$$



In order to find such a fit, we need to restrict ourselves to certain classes of functions f . With other words we need to assume a certain "model":

$$z_i \xrightarrow{f} y_i$$

In this course we will consider models of the following kind:

$$f : \mathbb{R} \rightarrow \mathbb{R}, \quad f(z) := \sum_{k=1}^n x_k f_k(z)$$

- More precisely, we assume that the relation between the z_i and the y_i can be modeled by a *linear combination* of some functions $f_k : \mathbb{R} \rightarrow \mathbb{R}$ with some coefficients/parameters x_k
- given by assumption* *to be determined* ($f(z_i) \cong y_i$)

(More generally $f, f_k : \mathbb{R}^k \rightarrow \mathbb{R}$. Important here is the fact that our model f is linear combined from the f_k .)

Example 1.41 (Polynomial Interpolation/Regression) One often considers a polynomial model:

$$f_k(z) := z^{k-1}, \quad \text{so that} \quad f(z) = x_1 + x_2 z + x_3 z^2 + \cdots + x_n z^{n-1}$$

For example, if $n = 2$ then $f(z) = x_1 + x_2 z$ (an affine linear model).

Exact: Interpolation

$$Ax = b$$

Approximate: Regression

$$Ax \approx b$$

A common approach to address a regression problem is a linear least squares formulation:

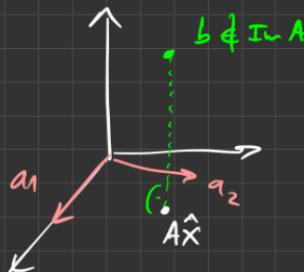
$$\begin{aligned}\min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2 &= \sum_{i=1}^m (Ax - b)_i^2 \\ &= \sum_{i=1}^m (f(z_i) - y_i)^2\end{aligned}$$



1.8.2 Existence and Uniqueness Analysis

Let us consider the following cases:

$$A = \begin{pmatrix} 1 & 1 \\ a_1 & a_2 \\ 1 & 1 \end{pmatrix} \in \mathbb{R}^{3 \times 2} \quad Ax = b$$



$$\hat{x} := \arg \min_{x \in \mathbb{R}^2} \|Ax - b\|_2^2$$

(no solution to $Ax = b$)



unique solution x^* , $Ax^* = b$



a solution x , $Ax = b$

Summary

Aim:

Given $A \in \mathbb{R}^{m \times n}$ ($m \neq n$ possible) and $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ such that $Ax = b$.

Here:

$m = \#$ equations = $\#$ measurements = length of the column vectors

$n = \#$ unknowns = $\#$ parameters = $\#$ columns

$$A = m \begin{pmatrix} & & & n \\ | & \cdots & | \\ a_1 & \cdots & a_n \\ | & & | \end{pmatrix}, \text{ with image } \text{Im}(A) = \{Ax : \in \mathbb{R}^n\} = \text{span}(a_1, \dots, a_n)$$

Let us define the solution set

$$S := \{x \in \mathbb{R}^n : Ax = b\} = f_A^{-1}(\{b\}),$$

then there are three possible states, namely,

$$|S| = \begin{cases} 0 & : \text{"no solution", if } b \notin \text{Im}(A) \\ 1 & : \text{"unique solution", if } b \in \text{Im}(A) \text{ and independent columns } (\ker(A) = \{0\}) \\ \infty & : \text{"infinitely many solutions", if } b \in \text{Im}(A) \text{ and dependent columns } (\ker(A) \neq \{0\}) \end{cases}$$

For a given b , observe the relations between image and existence as well as kernel and uniqueness. In fact, $b \in \text{Im}(A)$ decides if solutions exist and $\ker(A) = \{0\}$ gives the solutions' **uniqueness**.

1.9 More on Image and Kernel

Let us fix $\mathbb{F} = \mathbb{R}$ in this section. In this subsection we derive some more results on the kernel

$$\ker(A) = \{x \in \mathbb{R}^n : Ax = 0\} \subset \mathbb{R}^n$$

and the image

$$\text{Im}(A) = \{Ax : x \in \mathbb{R}^n\} \subset \mathbb{R}^m.$$

These results prove useful in later sections; in particular when we talk about the singular value decomposition.

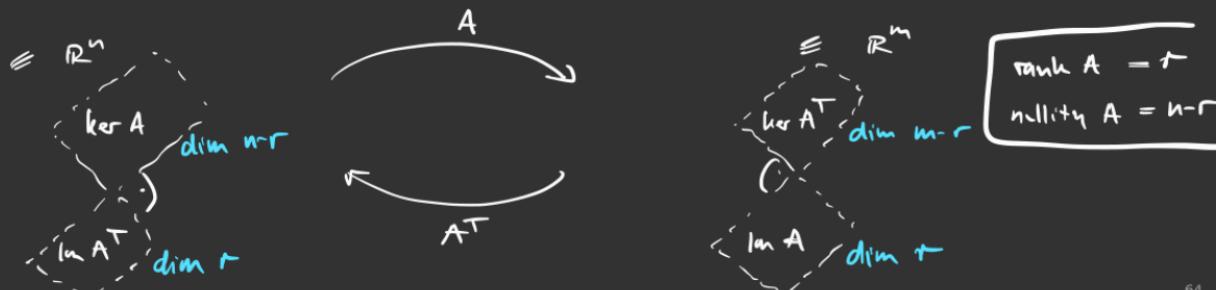
The Four Fundamental Subspaces

In the context of a matrix $A \in \mathbb{R}^{m \times n}$ there are four subspaces that stand out:

$$\ker(A) \perp \text{Im}(A^\top)$$

$$\text{Im}(A) \perp \ker(A^\top).$$

The big picture of linear algebra:



Example 1.42 Let us consider

$$A = \begin{pmatrix} 1 & 2 \\ 3 & 6 \end{pmatrix}, \quad A^\top = \begin{pmatrix} 1 & 3 \\ 2 & 6 \end{pmatrix}$$

Then we find

$$\text{Im}(A) = \text{span} \begin{pmatrix} 1 \\ 3 \end{pmatrix}$$

$$\ker(A) = \{x \in \mathbb{R}^2 : Ax = 0\}$$

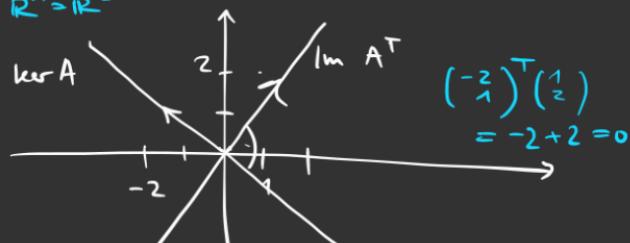
$$= \{x \in \mathbb{R}^2 : x_1 \begin{pmatrix} 1 \\ 3 \end{pmatrix} + x_2 \begin{pmatrix} 2 \\ 6 \end{pmatrix} = 0\}$$

$$= \{x \in \mathbb{R}^2 : 1x_1 + 2x_2 = 0\}$$

$$= \{x \in \mathbb{R}^2 : x_1 = -2x_2\}$$

$$= \text{span} \begin{pmatrix} -2 \\ 1 \end{pmatrix}$$

$$\Leftrightarrow \mathbb{R}^n \rightarrow \mathbb{R}^2$$



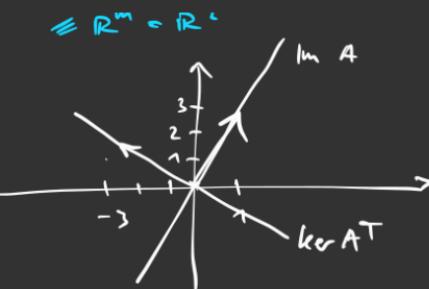
$$\text{Im}(A^\top) = \text{span} \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

$$\ker(A^\top) = \{x \in \mathbb{R}^2 : Ax = 0\}$$

$$= \{x \in \mathbb{R}^2 : 1x_1 + 3x_2 = 0\}$$

$$= \{x \in \mathbb{R}^2 : x_1 = -3x_2\}$$

$$= \text{span} \begin{pmatrix} -3 \\ 1 \end{pmatrix}$$



We need another definition:

Definition 1.43 (Orthogonal subspaces) Let $U, V \subset \mathbb{R}^n$ be two subspaces.

- i) We call U and V **orthogonal** ($U \perp V$) if $u^\top v = 0$ for all $u \in U, v \in V$.
- ii) We call

$$U^\perp := \{x \in \mathbb{R}^n : x^\top u = 0 \quad \forall u \in U\}$$

the **orthogonal complement** of V in \mathbb{R}^n .

Exercise: Show that $(U^\perp)^\perp = U$ and $U \perp U^\perp$.

Example 1.44

- i) $n = 2$, $U := \text{span}(\begin{pmatrix} 1 \\ 0 \end{pmatrix})$, $V := \text{span}(\begin{pmatrix} 0 \\ 1 \end{pmatrix})$. Then

$$\forall u = \begin{pmatrix} u_1 \\ 0 \end{pmatrix} \in U, v = \begin{pmatrix} 0 \\ v_2 \end{pmatrix} \in V : u^\top v = u_1 \cdot 0 + 0 \cdot v_2 = 0.$$

Thus, $U \perp V$.

- ii) $n = 3$, $U := \text{span}(\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}, \begin{pmatrix} 0 \\ 1 \\ 1 \end{pmatrix})$. Thus for any $u \in U$ we have $u = \begin{pmatrix} u_1 \\ u_2 \\ 0 \end{pmatrix}$. Then

$$\begin{aligned} U^\perp &= \{x \in \mathbb{R}^3 : x^\top u = 0 \quad \forall u \in U\} = \{x \in \mathbb{R}^3 : x_1 u_1 + x_2 u_2 = 0 \quad \forall u_1, u_2 \in \mathbb{R}\} \\ &= \{x \in \mathbb{R}^3 : x_1 = x_2 = 0\} \quad (\text{choose } u_1 = 1, u_2 = 0 \text{ and } u_1 = 0, u_2 = 1) \\ &= \text{span}(\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix}). \end{aligned}$$

[ex:draw pictures]

We now prove the orthogonality relation between the four fundamental subspaces:

Lemma 1.45 *Let $A \in \mathbb{R}^{m \times n}$. Then*

$$\text{Im}(A)^\perp = \ker(A^\top) \quad \text{and} \quad \ker(A)^\perp = \text{Im}(A^\top).$$

In words, $\ker(A^\top)$ is the orthogonal complement of $\text{Im}(A)$ in \mathbb{R}^m and $\text{Im}(A^\top)$ is the orthogonal complement of $\ker(A)$ in \mathbb{R}^n .

Proof. We show the first equation. The orthogonal complement of $\text{Im}(A)$ can be characterized as

$$\text{Im}(A)^\perp = \{y \in \mathbb{R}^m : z^\top y = 0 \quad \forall z \in \text{Im}(A)\} = \{y \in \mathbb{R}^m : x^\top A^\top y = 0 \quad \forall x \in \mathbb{R}^n\}. \quad (\text{simply write } z = Ax)$$

Now we show mutual subset relation. First,

$$\begin{aligned} y \in \text{Im}(A)^\perp &\Rightarrow \forall x \in \mathbb{R}^n : x^\top (A^\top y) = 0 \\ &\Rightarrow \text{for the basis vectors } e_1, \dots, e_n : e_i^\top (A^\top y) = (A^\top y)_i = 0 \\ &\Rightarrow A^\top y = 0 \text{ i.e., } y \in \ker(A^\top). \end{aligned}$$

Second,

$$\begin{aligned} y \in \ker(A^\top) &\Rightarrow A^\top y = 0 \\ &\Rightarrow \forall x \in \mathbb{R}^n : x^\top (A^\top y) = (Ax)^\top y = 0 \\ &\Rightarrow y \in \text{Im}(A)^\perp. \end{aligned}$$

The second equation follows from applying the first equation to $C = A^\top$ and $(U^\perp)^\perp = U$. □

In terms of the transpose matrix we find two more characterizations of the image and kernel:

Lemma 1.46 Let $A \in \mathbb{R}^{m \times n}$. Then

- i) $\ker(A) = \ker(A^\top A)$ (and $\ker(A^\top) = \ker(AA^\top)$),
- ii) $\text{Im}(A) = \text{Im}(AA^\top)$ (and $\text{Im}(A^\top) = \text{Im}(A^\top A)$).

Proof. We only prove i) here. We show this by mutual subset relation:

- " $\ker(A) \subseteq \ker(A^\top A)$ ":

$$\text{Let } x \in \ker(A) \xrightarrow{\text{Def. } \ker(A)} Ax = 0 \Rightarrow A^\top Ax = 0 \xrightarrow{\text{Def. } \ker(A^\top A)} x \in \ker(A^\top A).$$

- " $\ker(A^\top A) \subseteq \ker(A)$ ":

$$\text{Let } x \in \ker(A^\top A) \xrightarrow{\text{Def. }} A^\top Ax = 0 \Rightarrow \underbrace{x^\top A^\top Ax}_{= \|Ax\|_2^2} = 0 \xrightarrow{\text{norm } \|\cdot\|_2 \text{ is definite}} Ax = 0 \xrightarrow{\text{Def. }} x \in \ker(A).$$

Exercise: To prove ii) one can exploit the orthogonality of the subspaces as derived above.

The results for the transpose follow by applying the results to $C := A^\top$. □

Remark

The so-called Gram matrix $A^\top A$ plays a crucial role in many applications and also analysis, for instance

- it plays a key role to derive the singular value decomposition
- it is the system matrix in the normal equation $A^\top Ax = A^\top x$ for solving least squares problems
- in graph theory it appears as graph Laplacian
- if $A \approx \nabla$ (gradient), then $A^\top \approx \text{div}$ (divergence) and $A^\top A \approx \Delta$ (Laplacian)

A generalization of this result is given by the following lemma.

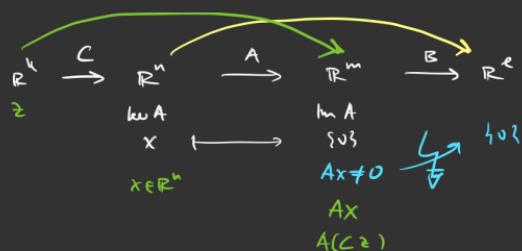
Lemma 1.47 Let $A \in \mathbb{R}^{m \times n}$. Then

- i) For a matrix $B \in \mathbb{R}^{\ell \times m}$ with $\ker(B) = \{0\}$ ("injective") we have

$$\ker(BA) = \ker(A).$$

- ii) For a matrix $C \in \mathbb{R}^{n \times k}$ with $\text{Im}(C) = \mathbb{R}^n$ ("surjective") we have

$$\text{Im}(AC) = \text{Im}(A).$$



Proof. We show mutual subset relation:

- i) " $\ker(BA) \subseteq \ker(A)$ ":

Let $BAx = B(Ax) = 0$. Since by assumption $\ker(B) = \{0\}$, we have $Ax = 0$.

- " $\ker(A) \subseteq \ker(BA)$ ":

For $Ax = 0$ we also have $BAx = B(Ax) = B0 = 0$.

- ii) " $\text{Im}(AC) \subseteq \text{Im}(A)$ ":

Let $y = ACx = A(Cx)$ for some $x \in \mathbb{R}^k$. Then with $z := Cx \in \mathbb{R}^n$ we see that $y = Az$ is in the image of A .

- " $\text{Im}(A) \subseteq \text{Im}(AC)$ ":

Let $y = Az$ for some $z \in \mathbb{R}^n$. Since $\text{Im}(C) = \mathbb{R}^n$ we find some coefficients $x \in \mathbb{R}^k$ so that $z = Cx$. With $y = ACx$ we see that y is in the image of AC . \square

Example

The typical context to apply Lemma ?? occurs when we have a decomposition of a matrix A and want to investigate its kernel and its image.

For example, consider the reduced QR decomposition $A = QR$, where $Q \in \mathbb{R}^{m \times n}$ contains orthonormal columns and $R \in \mathbb{R}^{n \times n}$ is upper triangular. Suppose that A has full rank, i.e., $\text{rank}(A) = n$, so that R is invertible (in particular $\text{rank}(R) = n$ and $\ker(R) = \{0\}$). We thus find by Lemma ?? i) that

$$\ker(A) = \ker(QR) = \ker(R) = \{0\}$$

and by Lemma ?? ii) that

$$\text{Im}(A) = \text{Im}(QR) = \text{Im}(Q).$$

With other words, the n columns in Q are an orthonormal basis for the image $\text{Im}(A)$ of A .

Solving Linear Systems (Direct Methods)

Recommended reading:

- Lectures in [4]: 6,7,8 for QR ; 20,21 for LU ; 23 for LL^\top
- Section I.4 in [3]
- Sections 2.6, 2.7 in [2]

References

- [1] R. Rannacher.
Numerik 0 - Einführung in die Numerische Mathematik.
Heidelberg University Publishing, 2017.
- [2] G. Strang.
Introduction to Linear Algebra.
Wellesley-Cambridge Press, 2003.
- [3] G. Strang.
Linear Algebra and Learning from Data.
Wellesley-Cambridge Press, 2019.
- [4] L.N. Trefethen and D. Bau.
Numerical linear algebra.
SIAM, Soc. for Industrial and Applied Math., Philadelphia, 1997.

2 Solving Linear Systems with Direct Methods

Aim:

*Given $A \in \mathbb{R}^{m \times n}$ ($m \neq n$ possible) and $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$ such that
 $Ax = b$.*

2.1 The Idea of “Factor and Solve”

A general theme in numerical mathematics is to reduce the general (possibly complicated) problem to one or more simpler problems with the help of transformations for which the property of interest is an invariant.

Simple cases:

- $A = D = \text{diag}(d_1, \dots, d_n)$ diagonal
- $A = L$ (or $A = U$) lower (or upper) triangular system
→ backward/forward substitution (exercise!)
- $A = Q$ orthogonal
→ $A^{-1} = Q^\top$
- A has special structure: tridiagonal/banded, Toeplitz, circulant,...

General case:

Assume $A = F_1 \cdots F_k$, where each factor $F_i \in \{D, L, U, Q\}$, then formally

$$x = F_k^{-1} \cdots F_1^{-1} b,$$

where each solving step F_i^{-1} can easily be performed.

(*Remark:* “direct” = finitely many steps to obtain the solution (typically operating on dense arrays))

Separate: Factorization and Solution!

- Since the *factorization* (*elimination/triangularization/orthogonalization*) step is typically much more expensive than the *solution* step, it makes sense to perform them separately, if the same matrix A is used for multiple right-hand sides b .
- The number of factors in a decomposition is the number of systems to be solved in the *solution* step.
From the factors we may also gain information about the
 - the image and kernel of A
 - invertibility of the matrix A in case $m = n$
 - solvability of the system (i.e., the cardinality $|S|$ of the solution set S)
- We will have a look at the following decompositions
 - $A = QR$ (two systems to be solved)
 - $A = P^T LU$ (three systems to be solved)
 - $A = LL^T$ (two systems to be solved)

Never compute the inverse!

- There are only very rare occasions, where an inverse matrix A^{-1} is needed. In most cases, one needs inverse matrix times a vector, i.e., $A^{-1}b$.
- For computing the inverse of an $(n \times n)$ -matrix A we have to solve n linear systems:

$$A \cdot [x_1, \dots, x_n] = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 0 & \ddots & \ddots & \vdots \\ \vdots & \ddots & \ddots & 0 \\ 0 & \cdots & 0 & 1 \end{pmatrix}, \quad (7)$$

where the $x_j \in \mathbb{R}^n$ are the unknown columns of the inverse of A . In practice, this is typically done by computing a factorization of A , which is then used to solve these n linear systems in (??) (see, e.g., the LAPACK routine `getri`).

- Thus, never do

```
x = inv(A) @ b
```

instead of

```
x = solve(A, b).
```

2.2 The Gram-Schmidt Algorithm and the QR decomposition

2.2.1 Projectors

For a fixed vector $x \in \mathbb{R}^n \setminus \{0\}$ we have derived the orthogonal projection onto its span by

$$\text{proj}_x(y) = \frac{x}{\|x\|_2} \cdot \frac{x^\top y}{\|x\|_2} = \frac{xx^\top}{x^\top x} \cdot y =: P_x y,$$

where $P_x := \frac{xx^\top}{x^\top x} \in \mathbb{R}^{n \times n}$.

We now collect some properties of this matrix:

- $\text{Im}(P_x) = \text{span}(x)$ (note that all columns are multiples of x) and thus $\text{rank}(P_x) = 1$
- P_x orthogonally projects a vector $y \in \mathbb{R}^n$ onto the linear subspace $\text{Im}(P_x) = \text{span}(x)$
- Idempotent:

$$P_x^2 := P_x \cdot P_x = \frac{xx^\top}{x^\top x} \cdot \frac{xx^\top}{x^\top x} = \frac{x(x^\top x)x^\top}{(x^\top x)^2} = \frac{xx^\top}{x^\top x} = P_x.$$

→ In words: Projecting multiple times is the same as projecting once.

We make this a definition:

Definition 2.1 (Projector) A matrix $P \in \mathbb{R}^{n \times n}$ is called **projector** if $P^2 = P$.

Example 2.2 (*Projectors*)

- $x = (1, 0)^\top, P_x = \dots$
- $x = (1, 1)^\top, P_x = \dots$
- For $\alpha \in \mathbb{R}$ consider $P_\alpha = \begin{pmatrix} 1 & \alpha \\ 0 & 0 \end{pmatrix}$ (exercise sheet)

For any projector $P \in \mathbb{R}^{n \times n}$ we can show:

Lemma 2.3 (Projector Properties) Let $P \in \mathbb{R}^{n \times n}$ be such $P^2 = P$, then

- i) $\text{Im } P = \ker(I - P)$,
- ii) $\ker(P) \cap \ker(I - P) = \{0\}$,
- iii) $(I - P)$ is also a projector,
- iv) $\forall y \in \mathbb{R}^n \exists v \in \text{Im}(P), r \in \text{Im}(I - P): y = v + r$,
with other words, the mapping $\text{Im}(P) \times \text{Im}(I - P) \rightarrow \mathbb{R}^n, (v, r) \mapsto v + r$ is bijective.

Proof.

- i) \subseteq : For $y = Px$ we find $(I - P)y = Px - P^2x = 0$.
 \supseteq : For $y \in \ker(I - P)$ we have $y = (I - P + P)y = 0 + Py \in \text{Im}(P)$.
- ii) Let $Px = 0$ and $(I - P)x = 0$, then $x = (I - P + P)x = 0 + 0 = 0$.
- iii) $(I - P)^2 = I - 2P + P^2 = I - 2P + P = I - P$.
- iv) Let $y \in \mathbb{R}^n$.

Existence: Choose $v = Py \in \text{Im}(P)$ and $r = (I - P)y \in \text{Im}(I - P)$, then we find

$$v + r = Py + (I - P)y = y.$$

Uniqueness: We assume there is another pair $\tilde{v} \in \text{Im } P = \ker(I - P)$ and $\tilde{r} \in \text{Im}(I - P) = \ker(P)$ with $y = \tilde{v} + \tilde{r}$. Since the kernel of matrix is a linear subspace (therefore closed under linear combinations), also $(v - \tilde{v}) \in \ker(I - P)$ and $(r - \tilde{r}) \in \ker(P)$. Now observe $0 = y - y = v - \tilde{v} + r - \tilde{r}$. Multiplying with P yields

$$0 = P(v - \tilde{v}) + P(r - \tilde{r}) = P(v - \tilde{v}) \quad \Rightarrow \quad (v - \tilde{v}) \in \ker(P) \cap \ker(I - P) = \{0\}.$$

Multiplying with $I - P$ yields

$$0 = (I - P)(v - \tilde{v}) + (I - P)(r - \tilde{r}) = (I - P)(v - \tilde{v}) \quad \Rightarrow \quad (r - \tilde{r}) \in \ker(I - P) \cap \ker(P) = \{0\}.$$

Thus $v = \tilde{v}$ and $r = \tilde{r}$.

Remark:

In view of Lemma ?? iv) we say that \mathbb{R}^n is the direct sum of the subspaces $\text{Im}(P)$ and $\text{Im}(I - P)$. Each vector $y \in \mathbb{R}^n$ uniquely splits into the additive components v and r . Due to i) and iii) of this lemma, also the same is true for the subspaces $\text{Im}(P)$ and $\ker(P)$.

We now continue with properties of P_x : Symmetry:

$$P_x^\top = \frac{(xx^\top)^\top}{x^\top x} = \frac{(x^\top)^\top x^\top}{x^\top x} = \frac{xx^\top}{x^\top x} = P_x.$$

In general we define:

Definition 2.4 (Orthogonal Projector) A matrix $P \in \mathbb{R}^{n \times n}$ is called **orthogonal projector** if $P^2 = P$ and $P^\top = P$.

For any orthogonal projector (such as P_x) one can show:

Lemma 2.5 (Orthogonal Projector Properties) Let $P \in \mathbb{R}^{n \times n}$ be such $P^2 = P$ and $P^\top = P$, then

$$\text{Im } P \perp \text{Im}(I - P).$$

Proof. From Lemma ?? and Lemma ?? (1.45) as well as the symmetry of P (and thus $I - P$) we find

$$\text{Im}(P) = \ker(I - P) = \ker((I - P)^\top) = \text{Im}(I - P)^\perp.$$

□

In view of Lemma ?? iv) we find for an orthogonal projector, that the components $v \in \text{Im}(P)$ and $r \in \ker(P)$ are orthogonal to each other.

Orthogonal Projection with Orthonormal Basis

Let us now consider more than just one vector. In fact, let $q_1, \dots, q_r \in \mathbb{R}^m$ be orthonormal; thus $r \leq m$. Then let us define the matrices

$$\begin{aligned}\hat{Q} &:= [q_1, \dots, q_r] \in \mathbb{R}^{m \times r}, \\ P := P_{q_1, \dots, q_r} &:= \hat{Q}\hat{Q}^\top \in \mathbb{R}^{m \times m}.\end{aligned}$$

Attention: For $r < m$, \hat{Q} is not an orthogonal matrix and thus $P = \hat{Q}\hat{Q}^\top \neq I$ in general. However, for the Gramian matrix which collects all possible pairs of inner products we have $\hat{Q}^\top \hat{Q} = I$ (\hat{Q}^\top is only a left-inverse).

We find the following properties of $P = P_{q_1, \dots, q_r}$:

- Sum of rank-one (orthogonal) projectors:

$$P = \sum_{j=1}^r q_j q_j^\top = \sum_{j=1}^r P_{q_j}.$$

- Orthogonal projector:

$$\begin{aligned}P^2 &= \hat{Q}(\hat{Q}^\top \hat{Q})\hat{Q}^\top = \hat{Q}\hat{Q}^\top = P \\ P^\top &= (\hat{Q}\hat{Q}^\top)^\top = (\hat{Q}^\top)^\top \hat{Q}^\top = P\end{aligned}$$

- P projects on the image of \hat{Q} : In fact, by Lemma ?? (1.47) ii) (with $\text{Im}(\hat{Q}^\top) = \mathbb{R}^r$) we find

$$\text{Im}(P) = \text{Im}(\hat{Q}\hat{Q}^\top) = \text{Im}(\hat{Q}).$$

In particular: $\text{rank}(P) = r$.

- By Lemma ?? i)+iii) and Lemma ??(1.47) i) (with $\ker(\widehat{Q}) = \{0\}$) we find

$$\text{Im}(I - P) = \ker(P) = \ker(\widehat{Q}\widehat{Q}^\top) = \ker(\widehat{Q}^\top)$$

- In Lemma ?? we recover Lemma ?? (1.45):

$$\text{Im}(P) \perp \text{Im}(I - P) \quad \Leftrightarrow \quad \text{Im}(\widehat{Q}) \perp \ker(\widehat{Q}^\top)$$

- By Lemma ?? iv) we have

$$\forall y \in \mathbb{R}^n \exists_1 v \in \text{Im}(P) = \text{Im}(\widehat{Q}), r \in \text{Im}(I - P) = \ker(\widehat{Q}^\top):$$

$$\begin{aligned} y &= v + r \\ &= Py + (I - P)y \\ &= \widehat{Q}\widehat{Q}^\top y + (I - \widehat{Q}\widehat{Q}^\top)y \end{aligned}$$

where v is the orthogonal projection of y onto $\text{Im}(\widehat{Q})$ and r the orthogonal residual vector; the components are orthogonal, i.e.,

$$(v, r) = v^\top r = 0.$$

Example 2.6 Let us consider:

$$q_1 = \frac{1}{\sqrt{2}}(1, 1, 0)^\top, q_2 = \frac{1}{\sqrt{2}}(-1, 1, 0), y = (0, 1, 1)^\top \in \mathbb{R}^3$$

Then

$$P = \widehat{Q}\widehat{Q}^\top = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

So that for $y = (y_1, y_2, y_3)^\top \in \mathbb{R}$ we obtain

$$Py = \begin{pmatrix} y_1 \\ y_2 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix},$$

i.e., as expected the orthogonal projection onto the x_1/x_2 -plane ($=\text{Im}(\widehat{Q})$).

Orthogonal Projection with Arbitrary Basis

Let a_1, \dots, a_n be linearly independent vectors in \mathbb{R}^m ($m \geq n$) and let us put the vectors into a matrix $A = [a_1, \dots, a_n] \in \mathbb{R}^{m \times n}$.

How to define an orthogonal projector on the image of A ?

Let us first recall that $\text{Im}(A) \perp \ker(A^\top)$ by Lemma ?? (1.45). Thus we are looking for a matrix $P \in \mathbb{R}^{m \times m}$ such that

$$\begin{aligned}\forall b \in \mathbb{R}^m: Pb &\in \text{Im}(A), \text{ i.e., } Pb = Ax \text{ for some } x \text{ to be determined} \\ b - Pb &\in \text{Im}(A)^\perp = \ker(A^\top)\end{aligned}$$

Combining these two gives

$$0 = A^\top(b - Pb) = A^\top(b - Ax) = A^\top b - A^\top Ax.$$

Then by Lemma ?? (1.46) i) we have $\ker(A^\top A) = \ker(A) = 0$, so that the Gram matrix $A^\top A$ is invertible, which yields

$$x = (A^\top A)^{-1} A^\top b$$

and the orthogonal projection b onto the image of A is given by

$$Ax = A(A^\top A)^{-1} A^\top b =: Pb.$$

Indeed we find, $P^2 = P$ and $P^\top = P$. Also note that for $A = \hat{Q}$ this collapses to $P = \hat{Q}\hat{Q}^\top$. Further note that this coincides with $P_x = x(x^\top x)^{-1}x^\top$.

Remark: The final step to bridge between orthogonal projections and least squares, is to show the intuitive result that orthogonal projections are precisely those projections that produce the smallest residual $(I - P)b$. This is shown later in this course.

Example 2.7 Let us consider:

$$a_1 = (1, 1, 0)^\top, a_2 = (0, 1, 0), y = (0, 1, 1)^\top \in \mathbb{R}^3.$$

We observe that $\text{Im}(A) = \text{Im}(\widehat{Q})$, so that we would expect the same projector as in the example above.

First we compute

$$A^\top A = \begin{pmatrix} 2 & 1 \\ 1 & 1 \end{pmatrix}.$$

From

$$A^\top Ax = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Leftrightarrow x = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and

$$A^\top Ax = \begin{pmatrix} 0 \\ 1 \end{pmatrix} \Leftrightarrow x = \begin{pmatrix} -1 \\ 2 \end{pmatrix}$$

we find

$$(A^\top A)^{-1} = \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix}.$$

And thus

$$P = A(A^\top A)^{-1}A^\top = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix}.$$

2.2.2 A=QR from the (classical) Gram–Schmidt Algorithm

- Aim: ultimately we want a decomposition of A in the following form:

[we "orthogonalize" the columns of A]

$$A = QR$$

$$\begin{bmatrix} \text{III} \end{bmatrix} = \begin{bmatrix} \text{III} \end{bmatrix} \begin{bmatrix} \text{I} & \text{II} \end{bmatrix}$$

↑ upper triangular

orthogonal
(orthonormal)
columns

$$\left[\text{span}(a_1, \dots, a_n) = \text{span}(q_1, \dots, q_n) \right]$$

$\left(\begin{array}{c} \{q_1, \dots, q_n\} \\ \text{for the column spaces} \end{array} \right)$

$$\Leftrightarrow \begin{aligned} 1: \quad a_1 &= r_{11} q_1 & \|q_j\| &= 1 \\ 2: \quad a_2 &= r_{12} q_1 + r_{22} q_2 & q_j^T q_i &= \delta_{ji} \\ &\vdots & & \\ k: \quad a_k &= r_{1k} q_1 + \dots + r_{kk} q_k & & \end{aligned}$$



$$\begin{aligned} 1: \quad q_1 &= \frac{1}{r_{11}} \cdot a_1, \quad 1 = \|q_1\| = \frac{1}{|r_{11}|} \|a_1\| \Leftrightarrow r_{11} = \pm \|a_1\| \\ 2: \quad q_2 &= \frac{1}{r_{22}} (a_2 - r_{12} q_1) = \frac{1}{r_{22}} (a_2 - r_{12} q_1) \end{aligned}$$

$$0 = q_1^T q_2 = \frac{1}{r_{22}} (a_2^T q_1 - r_{12}) \Leftrightarrow r_{12} = a_2^T q_1$$

$$1 = \|q_2\| = \frac{1}{|r_{22}|} \cdot \|a_2 - r_{12} q_1\|_2 \Leftrightarrow r_{22} = \pm \|a_2 - r_{12} q_1\|_2$$

⋮ ↑ "GRAM–SCHMIDT ORTHOGONALIZATION ALGORITHM"

Classical Gram–Schmidt Orthogonalization Algorithm

```
1  $r_{11} = \|a_1\|$ 
2  $q_1 = \frac{a_1}{r_{11}}$ 
3
4 for  $k = 2, \dots, n$  do
5   for  $\ell = 1, \dots, k-1$  do
6      $r_{\ell k} = a_k^\top q_\ell$ 
7   end
8    $\tilde{q}_k = a_k - \sum_{\ell=1}^{k-1} r_{\ell k} q_\ell = (I - P_{q_1, \dots, q_{k-1}}) a_k \in \text{Im}(\hat{Q}_{k-1})^\perp$ 
9    $r_{kk} = \|\tilde{q}_k\|$ 
10  if  $r_{kk} = 0$  then
11    pick arbitrary  $q_k \in \text{Im}(\hat{Q}_{k-1})^\perp = \ker(\hat{Q}_{k-1}^\top)$ 
12    // for example by solving  $\hat{Q}_{k-1}^\top q_k = 0$  and normalizing
13  end
14  else
15     $q_k = \frac{\tilde{q}_k}{r_{kk}}$ 
16  end
17 end
18 // For full QR:
19 Fill up columns of  $\hat{Q} := \hat{Q}_n$  with  $(m-n)$  orthonormal vectors of  $\ker(\hat{Q}_{k-1}^\top)$ 
20 Fill up rows of  $\hat{R} := (r_{ij})$  with  $(m-n)$  zero rows
```

Observation: This algorithm successively orthogonalizes the columns of A!

These ideas lead to

Theorem 2.8 (QR decomposition) Let $A \in \mathbb{R}^{m \times n}$ with $m \geq n$, then there exists a matrix $\widehat{Q} \in \mathbb{R}^{m \times n}$ with orthonormal columns and an upper triangular matrix $\widehat{R} \in \mathbb{R}^{n \times n}$ such that

$$A = \widehat{Q}\widehat{R}.$$

We call this the reduced QR decomposition of A .

One can extend the columns of \widehat{Q} with orthonormal columns to obtain an orthogonal matrix $Q \in \mathbb{R}^{m \times m}$ and the rows of \widehat{R} by zero rows to obtain a matrix $R = \begin{pmatrix} \widehat{R} \\ 0 \end{pmatrix} \in \mathbb{R}^{m \times n}$ and thereby obtain

$$A = QR.$$

We call this the **QR decomposition** of A .

Proof. Sketch: First note that by construction $\text{span}(a_1, \dots, a_k) = \text{span}(q_1, \dots, q_k)$ for all $1 \leq k \leq n$ and q_1, \dots, q_k orthonormal (exercise: verify this by an induction proof).

If $\ker(A) = \{0\}$ (independent columns), then for all $1 \leq k \leq n$ we have

$$a_k \notin \text{span}(a_1, \dots, a_{k-1}) = \text{span}(q_1, \dots, q_{k-1})$$

and thus for the residual of the projection

$$\tilde{q}_k = (I - P_{q_1, \dots, q_{k-1}})a_k \neq 0$$

so that $r_{kk} \neq 0$. Thus the classical Gram-Schmidt algorithms produces \widehat{Q} and \widehat{R} so that $A = \widehat{Q}\widehat{R}$.

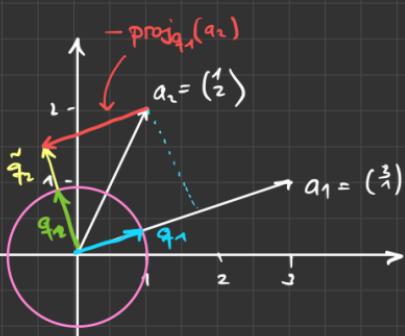
If columns of A are dependent, then there are k for which

$$a_k \in \text{span}(a_1, \dots, a_{k-1}) = \text{span}(q_1, \dots, q_{k-1})$$

so that the residual is $\tilde{q}_k = (I - P_{q_1, \dots, q_{k-1}})a_k = 0$, thus we pick an arbitrary vector in $q_k \in \text{Im}(\widehat{Q}_{k-1})^\perp = \ker(\widehat{Q}_{k-1}^\top)$ and continue. \square

Example 2.9

Let $A = \begin{pmatrix} 3 & 1 \\ 1 & 2 \end{pmatrix}$ with columns $a_1 = \begin{pmatrix} 3 \\ 1 \end{pmatrix}$ and $a_2 = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$



$$(a) \quad \hat{q}_1 := a_1 = \begin{pmatrix} 3 \\ 1 \end{pmatrix}, \quad \tilde{q}_1 := \frac{\hat{q}_1}{\|\hat{q}_1\|} = \frac{1}{\sqrt{10}} \cdot \begin{pmatrix} 3 \\ 1 \end{pmatrix}$$

Idea: Subtract from a_2 the projection of a_2 onto \tilde{q}_1

$$(b) \quad \tilde{q}_2 := a_2 - \text{proj}_{\tilde{q}_1}(a_2) = a_2 - a_2^T \tilde{q}_1 \cdot \tilde{q}_1 = \begin{pmatrix} 1 \\ 2 \end{pmatrix} - \left(\begin{pmatrix} 1 \\ 2 \end{pmatrix}^T \begin{pmatrix} 3 \\ 1 \end{pmatrix} \right) \cdot \frac{1}{\sqrt{10}} \cdot \begin{pmatrix} 3 \\ 1 \end{pmatrix}$$

$$= \begin{pmatrix} 1 \\ 2 \end{pmatrix} - \frac{5}{\sqrt{10}} \cdot \frac{1}{\sqrt{10}} \begin{pmatrix} 3 \\ 1 \end{pmatrix} = \begin{pmatrix} -0.5 \\ 1.5 \end{pmatrix}$$

$$\tilde{q}_2 := \frac{\tilde{q}_2}{\|\tilde{q}_2\|} = \underbrace{\frac{1}{\sqrt{2.5}}}_{\frac{\sqrt{2}}{\sqrt{5}}} \begin{pmatrix} -0.5 \\ 1.5 \end{pmatrix} = \frac{1}{\sqrt{10}} \cdot \begin{pmatrix} -1 \\ 3 \end{pmatrix}$$

$$\frac{\sqrt{2}}{\sqrt{5}} = \frac{2}{\sqrt{10}}$$

• We first observe:

$$q_1^T q_2 = \frac{1}{\sqrt{10}} \frac{1}{\sqrt{10}} \underbrace{\left(\begin{pmatrix} 3 \\ 1 \end{pmatrix}^T \begin{pmatrix} -1 \\ 3 \end{pmatrix} \right)}_{=0} = 0 \quad \checkmark$$

so that $\{q_1, q_2\}$:

- orthogonal \checkmark
- normalized \checkmark

• Now we write the numbers into matrices:

- goal: $A = Q \cdot R$, Q orthogonal, R triangular

- we define $Q := [q_1, q_2] = \frac{1}{\sqrt{10}} \begin{pmatrix} 3 & -1 \\ 1 & 3 \end{pmatrix} \Rightarrow$ orthogonal \checkmark

- How to define R ?

↳ from above: $r_{11} = \|q_1\| = \sqrt{10}$

$$r_{12} = q_2^T q_1 = 5 / \sqrt{10}$$

$$r_{22} = \|\tilde{q}_2\| = \frac{\sqrt{5}}{\sqrt{2}}$$

$$r_{21} = 0$$

- Let us verify:

$$Q \cdot R = \frac{1}{r_{10}} \begin{pmatrix} 3 & -1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} r_{10} & \frac{s}{r_{10}} \\ 0 & \frac{r_5}{r_2} \end{pmatrix} = \begin{pmatrix} 3 & \frac{1}{2} \cdot 3 - \frac{1}{2} \\ 1 & \frac{1}{2} \cdot 1 + 3 \cdot \frac{1}{2} \end{pmatrix}$$

↓ ↓ ↓

$\Rightarrow \begin{pmatrix} 1 & \frac{1}{2} \\ 0 & \frac{1}{2} \end{pmatrix}$

$= \begin{pmatrix} 3 & 1 \\ 1 & 2 \end{pmatrix} = A \checkmark$

- Extension to higher dimensions and more than 2 vectors:
 - Subtract the projections onto all previous q_k 's

\Rightarrow thereby we obtain the triangular structure for the coefficients put in the matrix R

Let $m \geq n$.

(1) Factorization

Gram-Schmidt orthogonalization algorithm, Householder reflections or Givens Rotations can be used.

In Python

$$Q, R = \text{scipy.linalg.qr}(A)$$

or for the reduced version run

$$\hat{Q}, \hat{R} = \text{scipy.linalg.qr}(A, \text{ mode}=\text{"economic"})$$

(2) Solving

Let us consider the reduced QR decomposition $\hat{Q}\hat{R} = A$. Then project b on the image of A by $\hat{Q}\hat{Q}^\top b$. Then we obtain the solvable auxiliary problem

$$Ax = \hat{Q}\hat{Q}^\top b \Leftrightarrow \hat{Q}\hat{R}x = \hat{Q}\hat{Q}^\top b \stackrel{\ker \hat{Q} = \{0\}}{\Leftrightarrow} \hat{R}x = \hat{Q}^\top b.$$

Note that if $b \in \text{Im}(A)$ then $b = \hat{Q}\hat{Q}^\top b$, so that in this case we solve the original problem

$$Ax = \hat{Q}\hat{Q}^\top b = b.$$

In Python

```
x = scipy.linalg.solve_triangular(R, Q.T @ b)
```

2.3 Gaussian Elimination and the *LU* Decomposition

(1) Factorization: Row elementary operations

Apply transformations to A (and b), which do not affect the solution x (more precisely the solution set S will not change), to bring A into a simple form and collect all transformations on the fly.

- the factorization **process** is known as *Gaussian Elimination*
- the **result** will be an invertible lower triangular matrix L , some sort of upper triangular matrix U and an orthogonal (more precisely a permutation) matrix P , such that

$$A = P^T \textcolor{orange}{LU}.$$

(2) Solve: Forward/Backward substitution

$$Ax = b \Leftrightarrow Ux = L^{-1}Pb$$

Example 1: Frobenius Matrices

$$A = \begin{pmatrix} 1 & 3 & 5 \\ 0 & 2 & 3 \\ 2 & 4 & 6 \end{pmatrix}, \quad b = \begin{pmatrix} 4 \\ 2 \\ 6 \end{pmatrix} \quad Ax = b \Leftrightarrow \begin{array}{l} x_1 + 3x_2 + 5x_3 = 4 \\ 2x_2 + 3x_3 = 2 \\ 2x_1 + 4x_2 + 6x_3 = 6 \end{array}$$

We apply the transformation: 1) scaling one row and adding it to another row

$$\begin{array}{c} \left(\begin{array}{ccc|c} 1 & 3 & 5 & 4 \\ 0 & 2 & 3 & 2 \\ 2 & 4 & 6 & 6 \end{array} \right) \xrightarrow{\text{III} \leftarrow \text{III}-2\text{I}} \left(\begin{array}{ccc|c} 1 & 3 & 5 & 4 \\ 0 & 2 & 3 & 2 \\ 0 & -2 & -4 & -2 \end{array} \right) \xrightarrow{\text{III} \leftarrow \text{III}+\text{II}} \left(\begin{array}{ccc|c} 1 & 3 & 5 & 4 \\ 0 & 2 & 3 & 2 \\ 0 & 0 & -1 & 0 \end{array} \right) \\ A|b \xrightarrow[L_1^{-1}]{ } L_1 A | L_1 b \xrightarrow[L_2^{-1}]{ } L_2 L_1 A | L_2 L_1 b \\ \text{III} \Rightarrow x_3 = 0 \\ \text{II} \Rightarrow x_2 = 1 \Rightarrow x = \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix} \\ \text{I} \Rightarrow x_1 = 1 \end{array}$$

Observation:

The transformations L_i can be written as:

$$L_1 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -2 & 0 & 1 \end{pmatrix}, \quad L_2 = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix}$$

Let us verify this for the first step

$$L_1 A = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ -2 & 0 & 1 \end{pmatrix} \begin{pmatrix} 1 & 3 & 5 \\ 0 & 2 & 3 \\ 2 & 4 & 6 \end{pmatrix} = \begin{pmatrix} 1 & 3 & 5 \\ 0 & 2 & 3 \\ 0 & -2 & -4 \end{pmatrix}, \quad L_1 b = \begin{pmatrix} 4 \\ 2 \\ -2 \end{pmatrix}$$

And since the transformations L_i are injective (independent columns), after the first step, we obtain an equivalent linear system:

$$Ax = b \Leftrightarrow L_1 A x = L_1 b$$

All in all:

By defining the upper triangular matrix $U := L_2 L_1 A$ and the lower triangular matrix $L := L_1^{-1} L_2^{-1}$ we find

$$A = LU.$$

In general:

If “ A permits”, we obtain:

$$\underbrace{(L_{n-1} \cdots L_2 L_1)}_{(\text{lower triangular + invertible})} \cdot A = U \quad \Leftrightarrow \quad A = LU, \quad L := (L_{n-1} \cdots L_2 L_1)^{-1}.$$

Note:

- The lower triangular structure in the matrices L_j is obtained by following a “top to bottom” approach.
- Thereby we also make sure that we ultimately obtain an “upper triangular” system.

Frobenius Matrices

$$\underbrace{\begin{pmatrix} 1 & 0 & & \cdots & 0 \\ 0 & 1 & 0 & & \vdots \\ 0 & \ddots & 0 & & \\ 0 & & 1 & 0 & \\ 0 & & \ell_{j+1,j} & \ddots & 0 \\ \vdots & \vdots & \vdots & 0 & 1 & 0 \\ 0 & \cdots & 0 & \ell_{m,j} & 0 & 0 & 1 \end{pmatrix}}_{=:L_j} \begin{pmatrix} --a_1-- \\ --a_2-- \\ \vdots \\ --a_j-- \\ \vdots \\ --a_m-- \end{pmatrix} = \begin{pmatrix} --a_1-- \\ \vdots \\ --a_j-- \\ \ell_{j+1,j}a_j + a_{j+1} \\ \vdots \\ \ell_{m,j}a_j + a_m \end{pmatrix}$$

- If L_j is defined in this way, then $\ell_{i,j}$ is the multiple for the j -th row which is then added to the i -th row.
- Since we want to produce zeroes underneath the diagonal element in our system, we choose

$$\ell_{i,j} = -\frac{a_{ij}}{a_{jj}} \quad (a_{jj} \neq 0).$$

→ We will now illuminate properties of such Frobenius matrices which come in handy when analyzing the Gaussian elimination procedure!

Properties

Lemma 2.10 Let $\ell_j := (0, \dots, 0, \ell_{j+1,j}, \dots, \ell_{m,j})^\top \in \mathbb{R}^m$, $e_j \in \mathbb{R}^m$ be the j -th unit vector and $I \in \mathbb{R}^{m \times m}$ be the identity matrix. Then the matrix

$$L_j := I + \ell_j e_j^\top \in \mathbb{R}^{m \times m}$$

satisfies:

- i) The matrix L_j is an invertible lower triangular matrix.
- ii) The inverse of L_j is given by $L_j^{-1} = I - \ell_j e_j^\top \in \mathbb{R}^{m \times m}$.
- iii) For $i \leq j$ it holds that $L_i L_j = I + \ell_j e_j^\top + \ell_i e_i^\top$ and $L_i^{-1} L_j^{-1} = I - \ell_j e_j^\top - \ell_i e_i^\top$.

Proof. i) First note that $\ell_j e_j^\top$ is a lower triangular matrix with zeroes on its diagonal because $\ell_{i,j} = 0$ for $i \leq j$. Therefore L_j is a lower triangular matrix with ones on its diagonal and thus invertible (see, e.g., $\det(L_j) = 1 \neq 0$).

ii) Since the inverse matrix is unique it is sufficient to show that $L_j(I - \ell_j e_j^\top) = I$. By inserting the definition we find that

$$\begin{aligned} L_j(I - \ell_j e_j^\top) &= (I + \ell_j e_j^\top)(I - \ell_j e_j^\top) = I + \ell_j e_j^\top - \ell_j e_j^\top - \ell_j e_j^\top \ell_j e_j^\top \\ &= I - \ell_j (\color{blue}{e_j^\top \ell_j}) e_j^\top \\ &= I, \end{aligned}$$

where we have exploited $e_j^\top \ell_j = 0$ which follows from $\ell_{j,j} = 0$.

iii) We insert definitions and compute the products. For the first product we get

$$\begin{aligned} L_i L_j &= (I + \ell_i e_i^\top)(I + \ell_j e_j^\top) = I + \ell_i e_i^\top + \ell_j e_j^\top + \ell_i e_i^\top \ell_j e_j^\top \\ &= I + \ell_i e_i^\top + \ell_j e_j^\top + \ell_i (\color{blue}{e_i^\top \ell_j}) e_j^\top \\ &= I + \ell_i e_i^\top + \ell_j e_j^\top, \end{aligned}$$

where we have exploited $e_i^\top \ell_j = 0$, which follows from $\ell_{i,j} = 0$ for all $i \leq j$. The second statement follows along the same lines. □

Example 2: Permutation Matrices

We now additionally allow for a second type of transformation: 2) row swap (= partial pivoting)

Let us now consider an example where the “top-to-bottom” approach would fail:

$$\left(\begin{array}{ccc|c} 0 & 2 & 3 & 2 \\ 1 & 3 & 5 & 4 \\ 2 & 4 & 6 & 6 \\ 1 & 5 & 8 & 6 \end{array} \right) \xleftrightarrow{\text{I} \leftrightarrow \text{II}} \left(\begin{array}{ccc|c} 1 & 3 & 5 & 4 \\ 0 & 2 & 3 & 2 \\ 2 & 4 & 6 & 6 \\ 1 & 5 & 8 & 6 \end{array} \right) \xrightarrow{\text{III}' = \text{III}-2\text{I}} \left(\begin{array}{ccc|c} 1 & 3 & 5 & 4 \\ 0 & 2 & 3 & 2 \\ 0 & -2 & -4 & -2 \\ 1 & 5 & 8 & 6 \end{array} \right) \xrightarrow{\text{IV}' = \text{IV}-\text{I}} \left(\begin{array}{ccc|c} 1 & 3 & 5 & 4 \\ 0 & 2 & 3 & 2 \\ 0 & -2 & -4 & -2 \\ 0 & 2 & 3 & 2 \end{array} \right)$$

$$P_{12} = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \quad L_1 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ -2 & 0 & 1 & 0 \\ -1 & 0 & 0 & 1 \end{pmatrix}$$

$$\begin{aligned} \text{III}' &= \text{III} + \text{II} \quad \left(\begin{array}{ccc|c} 1 & 3 & 5 & 4 \\ 0 & 2 & 3 & 2 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right) \Rightarrow x_1 = 1 \\ \text{IV}' &= \text{IV} - \text{II} \quad \left(\begin{array}{ccc|c} 1 & 3 & 5 & 4 \\ 0 & 2 & 3 & 2 \\ 0 & 0 & -1 & 0 \\ 0 & 0 & 0 & 0 \end{array} \right) \Rightarrow x_2 = 1 \\ &\qquad \qquad \qquad \Rightarrow x_3 = 0 \end{aligned}$$

$$L_2 = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & -1 & 0 & 1 \end{pmatrix}$$

Remark: The multiples from the Frobenius matrices can be stored in-place. We even store them with reverse sign, because we are interested in their inverses.

All in all:

$$L_2 L_1 P_{12} A = U \text{ is not upper triangular}$$

- We observe that U is not a “perfect” upper triangular matrix.
 - The structure of U is called Row Echelon Form (REF).
 - Any matrix $A \in \mathbb{R}^{m \times n}$ can be transformed into a matrix $U \in \mathbb{R}^{m \times n}$ of REF with the help of matrices P_{jk_j}, L_j from above.
- In order to reduce rounding errors one chooses the element in the current column which has largest absolute value as the pivot element by permuting rows first.
→ We do not further study stability issues in this course.

Permutation Matrices

Definition 2.11 (Permutation Matrix) A matrix $P \in \mathbb{R}^{m \times m}$ is called **permutation matrix**, if it has exactly one entry "1" in each row and column and zero otherwise.

In each step of the Gaussian elimination (with pivoting) we only swap two rows at a time: The matrix

$$P_{ik} = \begin{pmatrix} 1 & 0 & & \cdots & & 0 \\ 0 & \ddots & & & & \\ & & 1 & & & \\ & & & 0 & \cdots & 0 & 1 \\ & & & & 1 & & 0 \\ \vdots & & \vdots & & \ddots & & \vdots \\ & & 0 & & & 1 & \\ & & & 1 & 0 & \cdots & 0 \\ 0 & & & & \cdots & & 0 & 1 \end{pmatrix} \leftarrow i-th \\ \leftarrow k-th$$

swaps rows k and i , when multiplied from the left to a matrix.

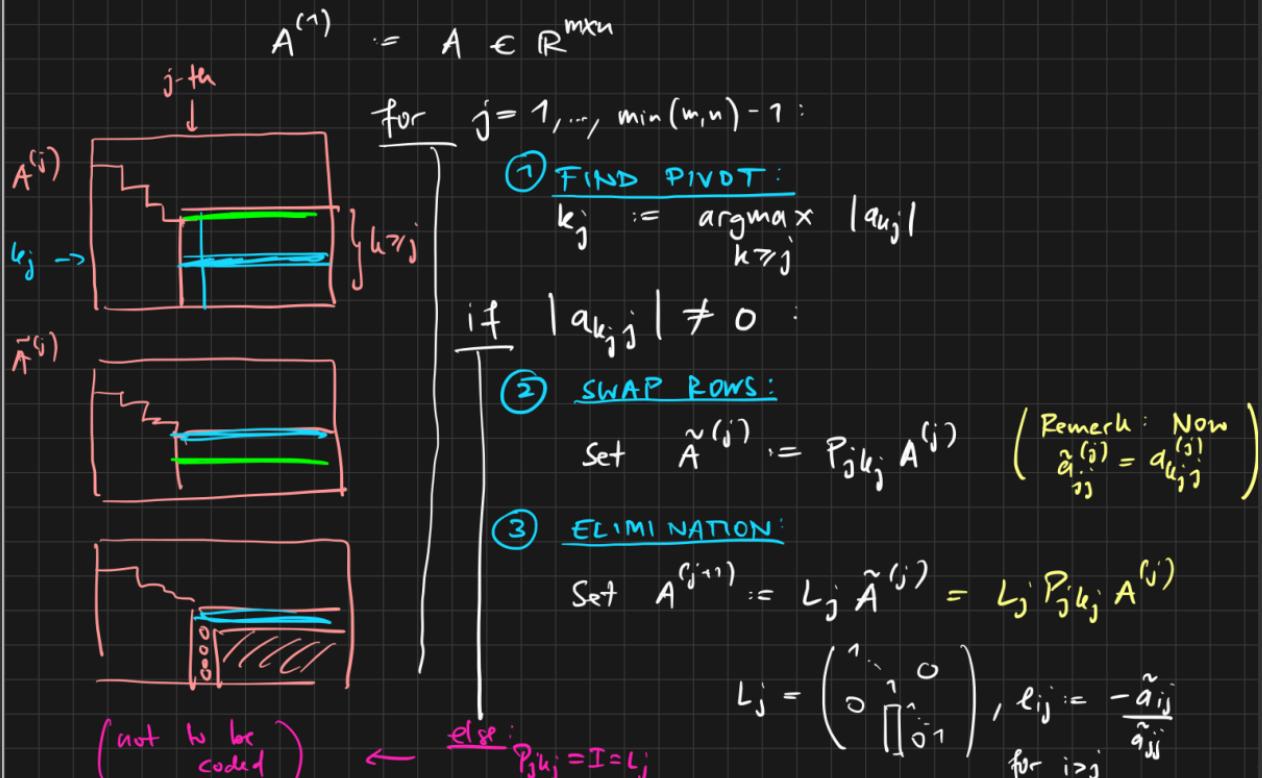
→ We illuminate further properties in the exercises.

Example 2.12 (Permutation Matrix) Consider $P := P_{23} \in \mathbb{R}^{3 \times 3}$, i.e.,

$$P = P_{23} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}.$$

- Multiply from the left to a matrix $A \in \mathbb{R}^{3 \times 3}$ and observe how it acts on the rows.
- Observe that $P^\top P = I$, so that $P^\top = P^{-1}$. Even $P^\top = P$, i.e., P is self-inverse.
- Derive its CSR format
 - `data = [1,1,1]`
 - `indices = [0,2,1]` \leftarrow *the only relevant information*
 - `indptr = [0,1,2,3]`

Algorithm: Elimination with row pivoting



Remark: We can work *in-place* and store numbers for L and U in the same array.

In-place Gaussian Elimination with Row Pivoting (for $m = n$)

INPUT: $A \in \mathbb{R}^{n \times n}$ (and $b \in \mathbb{R}^n$)

OUTPUT: LU decomposition $PA = LU$ (and if $Ax = b$ is uniquely solvable the solution $x \in \mathbb{R}^n$)

```
1 # FACTORIZATION
2 initialize piv = [1,2,...,n]
3 for j = 1,...,n - 1 do
4     # Find the j-th pivot
5      $k_j := \arg \max_{k \geq j} |a_{kj}|$ 
6     if  $a_{kj} \neq 0$  then
7         # Swap rows
8         A[kj,:]  $\leftrightarrow$  A[j,:]
9         # by hand we also transform b on the fly
10        b[kj]  $\leftrightarrow$  b[j]
11        piv[kj]  $\leftrightarrow$  piv[j]
12        # Elimination
13        for k = j + 1,...,n do
14             $\ell_{kj} := a_{kj}/a_{jj}$ 
15             $a_{kj} = \ell_{kj}$ 
16            for i = j + 1,...,n do
17                 $a_{ki} = a_{ki} - \ell_{kj}a_{ji}$ 
18            end
19            # by hand we also transform b on the fly
20             $(b_k = b_k - \ell_{kj}b_j)$ 
21        end
22    end
23 end
24 # SOLVE
25 ...
```

As in the algorithm consider $A \in \mathbb{R}^{n \times n}$. Then the algorithm eventually leads to

$$U := A^{(n)} = L_{(n-1)} P_{(n-1)k_{(n-1)}} \dots L_3 P_{3k_3} L_2 P_{2k_2} L_1 P_{1k_1} A.$$

By construction of the algorithm, $A^{(n)} =: U$ has row echelon form (no rigorous proof provided in this course).

Question: Can we group all L_i and P_{ik_i} in such a way that $PA = LU$?

Lemma 2.13 Let $m \in \mathbb{N}$. Let $P_{ik_i} \in \mathbb{R}^{m \times m}$ be the permutation matrix which results from interchanging the i -th and k_i -th column of the identity matrix in $\mathbb{R}^{m \times m}$, where $k_i \geq i$. Further for $\ell_j := (0, \dots, 0, \ell_{j+1,j}, \dots, \ell_{m,j})^\top \in \mathbb{R}^m$ and the j -th unit vector $e_j \in \mathbb{R}^m$, let $L_j := I + \ell_j e_j^\top \in \mathbb{R}^{m \times m}$. Then show that for all $1 \leq j < i \leq k_i \leq m$ we have

$$P_{ik_i} L_j = \widehat{L}_j P_{ik_i}$$

where $\widehat{L}_j := I + (P_{ik_i} \ell_j) e_j^\top$.

Proof. We find

$$\begin{aligned} P_{ik_i} L_j &= P_{ik_i} (I + \ell_j e_j^\top) \\ &= P_{ik_i} + P_{ik_i} \ell_j e_j^\top \\ &= P_{ik_i} + P_{ik_i} \ell_j e_j^\top P_{ik_i}^\top P_{ik_i} \\ &= (I + P_{ik_i} \ell_j e_j^\top P_{ik_i}^\top) P_{ik_i} \\ &= (I + P_{ik_i} \ell_j (P_{ik_i} e_j)^\top) P_{ik_i} \\ &= (I + P_{ik_i} \ell_j e_j^\top) P_{ik_i}. \end{aligned}$$

Since $j < i \leq k_i$ we find that $P_{ik_i} e_j = e_j$, since only zeroes are swapped. □

By applying this result multiple times, we obtain

$$\underbrace{(\hat{L}_{n-1} \cdots \hat{L}_2 \hat{L}_1)}_{=: \hat{L}} \underbrace{(P_{(n-1)k_{(n-1)}} \cdots P_{2k_2} P_{1k_1})}_{=: P} \cdot A = U$$
$$L \stackrel{=: \hat{L}^{-1}}{\Leftrightarrow} PA = LU.$$

Summary: Row echelon form and LU decomposition

Definition 2.14 (REF)

a) **Row elementary operations** are

- 1) add a nonzero multiple of one row to another
- 2) swap two rows

b) **A matrix is in row echelon form (REF)** when it satisfies the following conditions:

- 1) The first non-zero element in each row (called the leading entry) is in a column to the right of the leading entry in the previous row.
- 2) Rows with all zero elements, if any, are below rows having a non-zero element.

By applying these types of operations we find:

Theorem 2.15 (LU Decomposition) Every matrix $A \in \mathbb{F}^{m \times n}$ can be transformed to REF by row elementary operations. Thus there is a matrix $U \in \mathbb{F}^{m \times n}$ in REF, a lower triangular matrix $L \in GL(m, \mathbb{F})$ with $\ell_{ij} = 0, \forall j > i$, and $\ell_{ii} = 1, \forall i$, and a permutation matrix $P \in GL(m, \mathbb{F})$ with exactly one entry "1" in each row and column and zero otherwise, such that

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

Since triangular matrices are invertible if and only if the diagonal elements are nonzero, we find for the square case $m = n$, that:

Corollary 2.16 (Invertibility of A) A matrix $A \in \mathbb{F}^{n \times n}$ is invertible, if and only if its REF $U \in \mathbb{F}^{n \times n}$ has a nonzero diagonal, i.e., $u_{ii} \neq 0, \forall i = 1, \dots, n$.

(1) Factorization: $\text{Lu, Piv} = \text{scipy.linalg.lu_factor}(A)$

- determine factors L, U and permutation matrix P such that $LU = PA$
- the factors L, U are compactly stored in one matrix $\text{Lu} \in \mathbb{R}^{n \times n}$ of the same size as A and the permutation matrix P in CSR format as integer vector $\text{Piv} \in \mathbb{N}^n$.

(2) Solution: $x = \text{scipy.linalg.lu_solve}((\text{Lu}, \text{Piv}), b)$

(2.1) permute right-hand side $\bar{b} = Pb$

(2.2) solve lower triangular system $Lz = \bar{b}$ for z (forward substitution)

(2.3) solve REF system $Ux = z$ for x (backward substitution)

Both, (1) and (2), are combined in the routine

$x = \text{scipy.linalg.solve}(A, b).$

2.3.1 Identify the number of solutions from the REF

First, by inserting the LU decomposition we obtain

$$S := \{x \in \mathbb{R}^n : Ax = b\} \stackrel{A=P^T LU}{=} \{x \in \mathbb{R}^n : P^T L U x = b\} = \{x \in \mathbb{R}^n : Ux = \underbrace{L^{-1} Pb}_{=: z}\}.$$

Then we find for the three possible cases of the solution set (exercise):

- 1) U does not have a zero row (i.e., $m \leq n$)

1.1) $m = n$: Then U is invertible and $|S| = 1$ with $x = U^{-1}L^{-1}Pb$

1.2) $m < n$: Then has dependent columns but $\text{Im}(U) = \mathbb{R}^m$, so that $|S| = \infty$

Note: The m rows of U are independent. Thus $m = \dim \text{Im } U^\top$. Also from dimension formula

$\dim \ker U^\top = m - \dim \text{Im } U^\top = 0$, so that $\ker U^\top = \{0\}$ and thus $\text{Im}(U) = (\ker U^\top)^\perp = \{0\}^\perp = \mathbb{R}^m$.

- 2) U has at least one zero row

2.1) For all zero rows in U , the transformed right-hand side z is also zero there:

$\Rightarrow Ux = z$ has infinitely many solutions, i.e., $|S| = \infty$

(Note: $0x_1 + \dots + 0x_n = z_i = 0$ is true for any x)

2.2) else: $|S| = 0$

(Note: $0x_1 + \dots + 0x_n = z_i \neq 0$ false for any x)

2.4 The Cholesky Decomposition

For symmetric and positive definite matrices $A \in \mathbb{R}_{\text{spd}}^{n \times n} \subset \text{GL}_n(\mathbb{R})$ we obtain the following improvement:

Theorem 2.17 *We have the equivalence*

$$A \in \mathbb{R}_{\text{spd}}^{n \times n} \Leftrightarrow \exists_1 L \in \mathbb{R}^{n \times n} \text{ lower triangular, } l_{ii} > 0: A = LL^\top.$$

- The Decomposition $A = LL^\top$ is called the **Cholesky decomposition of A** .
- Named after the french Mathematician André-Louis Cholesky (1875-1918) who developed this decomposition during his surveying work to solve the normal equation $A^\top Ax = A^\top b$.
- We can derive an algorithm to compute the factor L .
- **Solving using $A = LL^\top$**

$$Ax = b \Leftrightarrow LL^\top x = b \Leftrightarrow Lz = b, L^\top x = z \quad (\text{forward/backward Subst.})$$

In Python:

(1) **Factorization:** `L, lower = scipy.linalg.cho_factor(A)`

(2) **Solution:** `x = scipy.linalg.cho_solve((L, lower), b)`

Numerical Comparison: LU vs. Cholesky

- **Computational Costs:**

The Cholesky decomposition is roughly twice as fast as Gaussian elimination (in terms of number of floating point operations). Clearly, we only need to compute one instead of two factors.

- **Stability (=“robustness against rounding errors”)** :

- Gaussian Elimination: Is only stable if a pivoting strategy is applied.
- Cholesky: Is stable even without pivoting.

(To avoid square roots, one can compute the LDL decomposition)

All in all:

*For symmetric and positive definite matrices (of moderate size),
the Cholesky factorization is the preferred algorithm!*

Eigenvalues: Theory and Algorithms

Recommended reading:

- Lectures 24, 25, 27 in [4]
- Sections I.6 in [3]
- Sections 6.1, 6.2, 6.4 in [2]
- Kapitel 7 in [1]

Literature:

[1] R. Rannacher.

Numerik 0 - Einführung in die Numerische Mathematik.

Heidelberg University Publishing, 2017.

[2] G. Strang.

Introduction to Linear Algebra.

Wellesley-Cambridge Press, 2003.

[3] G. Strang.

Linear Algebra and Learning from Data.

Wellesley-Cambridge Press, 2019.

[4] L.N. Trefethen and D. Bau.

Numerical linear algebra.

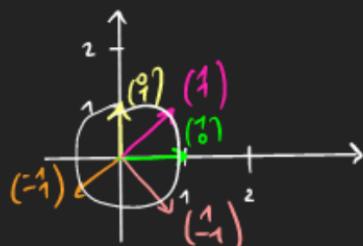
SIAM, Soc. for Industrial and Applied Math., Philadelphia, 1997.

3 Eigenvalues: Theory and Algorithms

3.1 Introduction

Example 3.1 (Illustration in 2d: Part 1)

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

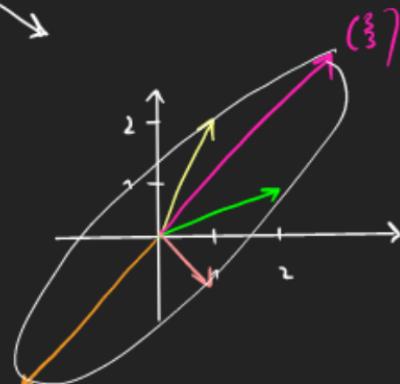


$$A \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

$$A \cdot \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

$$A \cdot \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 3 \\ 3 \end{pmatrix} = 3 \cdot \underbrace{\begin{pmatrix} 1 \\ 1 \end{pmatrix}}_{\text{eigenvector to the eigenvalue } 3}$$

$$A \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} -3 \\ 3 \end{pmatrix} = 3 \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$



$$A \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix} = 3 \cdot \begin{pmatrix} -1 \\ 1 \end{pmatrix}$$

↑
eigenvector for
the eigenvalue
3

3.2 Eigenvalues and Eigendecomposition

Definition 3.2 (Eigenvalues and -vectors) Let $A \in \mathbb{F}^{n \times n}$ be a matrix. A number $\lambda \in \mathbb{C}$ is called an **eigenvalue** of A , if

$$\exists v \in \mathbb{F}^n, v \neq 0: Av = \lambda v.$$

In that case, v is called an **eigenvector** and (λ, v) an **eigenpair**. The set of all eigenvalues is denoted by

$$\sigma(A) := \{\lambda \in \mathbb{C}: \lambda \text{ is eigenvalue of } A\}$$

and called the **spectrum of A** .

- 1) Assume we knew an eigenvalue λ :

Then we find a corresponding eigenvector by solving the linear equation

$$(A - \lambda I_n)v = 0$$

Observation:

$$v \text{ eigenvector} \Rightarrow \alpha v \text{ eigenvector } \forall \alpha \in \mathbb{F}$$

We often normalize the eigenvector by $\frac{v}{\|v\|_2}$.

- 2) Assume we had an eigenvector v :

Then the corresponding eigenvalue is uniquely determined by the so-called *Rayleigh-Quotient*

$$\lambda = \frac{v^T A v}{v^T v}$$

The determinant and eigenvalues

Let $A \in \mathbb{F}^{n \times n}$. Then:

1) Relation between the determinant and eigenvalues:

$$\begin{aligned}\lambda \in \mathbb{C} \text{ eigenvalue of } A &\Leftrightarrow \exists v \neq 0: Av = \lambda v \Leftrightarrow \exists v \neq 0: (A - \lambda I_n)v = 0 \\ &\Leftrightarrow \exists v \neq 0: v \in \ker(A - \lambda I_n) \Leftrightarrow (A - \lambda I_n) \text{ not injective} \\ &\Leftrightarrow (A - \lambda I_n) \notin \mathrm{GL}(n, \mathbb{F}) \Leftrightarrow \det(A - \lambda I_n) = 0\end{aligned}$$

2) Implication:

By invoking the Laplace formula (see Def.??) for the determinant we can show that the function

$$\lambda \mapsto \chi_A(\lambda) := \det(A - \lambda I_n)$$

is a **polynomial of degree $\leq n$** . Thus, we can state:

The eigenvalues of A are the roots of the polynomial $\chi_A(\lambda)$.

The fundamental theorem of algebra then assures the existence of eigenvalues (at most n distinct ones).

Definition: The polynomial $\chi_A(\lambda)$ is called **characteristic polynomial of A** .

Example 3.3 (Illustration in 2d: Part 2)

Let us consider the (2×2) matrix

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$$

from Example ?? above.

- We compute its eigenvalues by solving the following root finding problem:

$$\begin{aligned} 0 = \chi_A(\lambda) &= \det(A - \lambda I) = \det \left(\begin{pmatrix} 2 - \lambda & 1 \\ 1 & 2 - \lambda \end{pmatrix} \right) = (2 - \lambda)^2 - 1 \\ \Leftrightarrow \lambda &\in \{3, 1\} =: \{\lambda_1, \lambda_2\} = \sigma(A) \end{aligned}$$

- Now that we have the eigenvalues we can find corresponding eigenvectors by solving the following homogeneous linear systems:
 - For $\lambda_1 = 3$:

$$(A - \lambda_1 I)v^1 = 0 \Leftrightarrow \begin{pmatrix} -1 & 1 \\ 1 & -1 \end{pmatrix}v^1 = 0 \Rightarrow v_1^1 - v_2^1 = 0$$

Thus, the set of all eigenvectors corresponding to the eigenvalue λ_1 is given by

$$E(\lambda_1) := \{v \in \mathbb{R}^2 : Av = \lambda_1 v\} = \{v \in \mathbb{R}^2 : v_1^1 = v_2^1\} = \left\{ \begin{pmatrix} \alpha \\ \alpha \end{pmatrix} \in \mathbb{R}^2 : \alpha \in \mathbb{R} \right\} = \text{span} \left(\begin{pmatrix} 1 \\ 1 \end{pmatrix} \right)$$

Sometimes it is reasonable to choose eigenvectors of length 1, so that we normalize: $v^1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$

- For $\lambda_2 = 1$:

$$(A - \lambda_2 I)v^2 = 0 \Leftrightarrow \begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} v^2 = 0 \Leftrightarrow v_1^2 + v_2^2 = 0$$

Thus, the set of all eigenvectors corresponding to the eigenvalue λ_2 is given by

$$E(\lambda_2) := \{v \in \mathbb{R}^2 : Av = \lambda_2 v\} = \{v \in \mathbb{R}^2 : v_1^2 = -v_2^2\} = \left\{ \begin{pmatrix} \alpha \\ -\alpha \end{pmatrix} \in \mathbb{R}^2 : \alpha \in \mathbb{R} \right\} = \text{span} \left(\begin{pmatrix} 1 \\ -1 \end{pmatrix} \right)$$

Normalization: Choose $v^2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$

Remark:

The set of all eigenvectors corresponding to the eigenvalue $\lambda \in \sigma(A)$, i.e.,

$$E(\lambda) = \ker(A - \lambda I) \subset \mathbb{F}^n$$

is called **eigenspace to the eigenvalue λ of A** .

Lemma 3.4 (Matrix and Eigenvalue Properties)

- i) *Power of a matrix:* $A \in \mathbb{F}^{n \times n}$, $\lambda \in \sigma(A) \Rightarrow \lambda^k \in \sigma(A^k)$ for any $k \in \mathbb{N}$
- ii) *Inverse matrix:* $A \in GL_n(\mathbb{F})$, $\lambda \in \sigma(A) \Rightarrow \lambda \neq 0$, $\frac{1}{\lambda} \in \sigma(A^{-1})$
- iii) *Scaling:* $A \in \mathbb{F}^{n \times n}$, $\lambda \in \sigma(A) \Rightarrow \alpha\lambda \in \sigma(\alpha A)$ for any $\alpha \in \mathbb{F}$
- iv) $A \in \mathbb{F}^{n \times n}$ hermitian ($A = A^H$) $\Rightarrow \sigma(A) \subset \mathbb{R}$.
- v) $Q \in \mathbb{F}^{n \times n}$ unitary ($Q^H Q = I$), $\lambda \in \sigma(Q) \Rightarrow |\lambda| = 1$
- vi) $A \in \mathbb{F}^{n \times n}$ positive definite (semi-definite) ($x^H A x > 0$ (≥ 0)) $\Leftrightarrow \forall \lambda \in \sigma(A): \lambda > 0$ ($\lambda \geq 0$)
- vii) *The eigenvalues of an upper (lower) triangular matrix are sitting on the diagonal.*
- viii) *Similarity transformation:* $A \in \mathbb{F}^{n \times n}$, $T \in GL_n(\mathbb{F}) \Rightarrow \sigma(A) = \sigma(T^{-1}AT)$
- ix) *Shifts:* $A \in \mathbb{F}^{n \times n}$, (λ, v) eigenpair of $A \Rightarrow \forall s \in \mathbb{F}: (\lambda + s, v)$ eigenpair of $A + sI$

Attention: The following rules do not hold in general:

- $\lambda \in \sigma(A), \mu \in \sigma(B) \not\Rightarrow (\lambda + \mu) \in \sigma(A + B)$
- $\lambda \in \sigma(A), \mu \in \sigma(B) \not\Rightarrow (\lambda \cdot \mu) \in \sigma(A \cdot B)$

Proof. Exercise. Here, we exemplary prove viii):

□

Diagonalizing a matrix

Let us consider a matrix $A \in \mathbb{F}^{n \times n}$ with eigenpairs $(\lambda_i, v_i) \in \mathbb{F} \times \mathbb{F}^n$, so that

$$Av_i = \lambda_i v_i, \quad \text{for } 1 \leq i \leq n.$$

Using matrix notation this can be written as

$$A \cdot \underbrace{\begin{pmatrix} | & | & & | \\ v_1 & v_2 & \cdots & v_n \\ | & | & & | \end{pmatrix}}_{=:V \in \mathbb{F}^{n \times n}} = \begin{pmatrix} | & | & & | \\ \lambda_1 v_1 & \lambda_2 v_2 & \cdots & \lambda_n v_n \\ | & | & & | \end{pmatrix} = \underbrace{\begin{pmatrix} | & & | \\ v_1 & \cdots & v_n \\ | & & | \end{pmatrix}}_{=:V \in \mathbb{F}^{n \times n}} \underbrace{\begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}}_{=: \Lambda \in \mathbb{F}^{n \times n}}$$

which is equivalent to

$$AV = V\Lambda.$$

If V is invertible (note that this is not necessarily the case!), then we can rearrange this into the following decomposition

$$V^{-1}AV = \Lambda \Leftrightarrow A = V\Lambda V^{-1}.$$

One central question arises: When is V invertible?

Let us first revisit the example from above (see Examples ?? and ??)

Example 3.5 (*Illustration in 2d: Part 3*)

Let us again consider the *real symmetric* matrix

$$A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix},$$

with eigenpairs

$$\lambda_1 = 3, v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad \lambda_2 = 1, v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}.$$

Assembling the normalized eigenvectors into the matrix V yields

$$V = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}.$$

Since for the columns we have

$$\begin{pmatrix} 1 \\ 1 \end{pmatrix}^T \begin{pmatrix} 1 \\ -1 \end{pmatrix} = 1 - 1 = 0$$

and by construction

$$\|v_1\|_2 = \frac{1}{\sqrt{2}} \underbrace{\left\| \begin{pmatrix} 1 \\ 1 \end{pmatrix} \right\|}_{=\sqrt{2}} = 1, \quad \text{and similarly } \|v_2\|_2 = 1,$$

we find that V is orthogonal and thus in particular invertible.

In the previous Example ?? the matrix V of eigenvectors turned out to be orthogonal. The next theorem states, that this is true for any real symmetric matrix.

Theorem 3.6 (Eigendecomposition of real symmetric matrices) For any symmetric matrix $A \in \mathbb{R}^{n \times n}$, there is an orthogonal matrix $Q \in \mathbb{R}^{n \times n}$ (i.e., $Q^\top Q = I$) such that

$$Q^\top A Q = \begin{pmatrix} \lambda_1 & & & \\ & \lambda_2 & & \\ & & \ddots & \\ & & & \lambda_n \end{pmatrix} =: \text{diag}(\lambda_1, \dots, \lambda_n) \quad (= \text{diagonal matrix})$$

and $\lambda_i \in \mathbb{R}, i \in \{1, \dots, n\}$, are the eigenvalues of A . The columns of Q are the normalized eigenvectors.

Proof. In the exercises we will prove this statement for the special case that the matrix has n distinct eigenvalues. The general proof is rather technical and can be found in any standard textbook. □

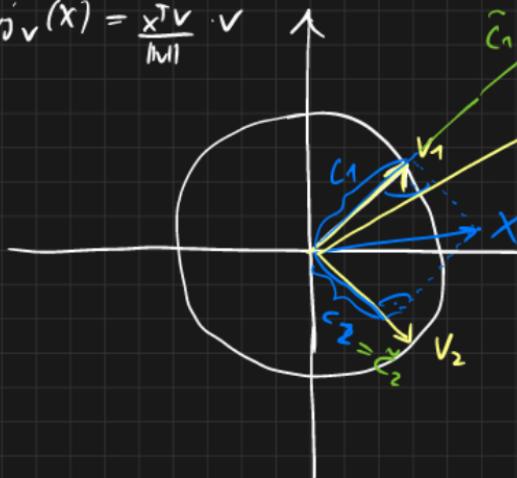
→ **Thus:** “knowing the eigenpairs = knowing the matrix”

An immediate consequence of Theorem ?? is this:

Corollary 3.7 A symmetric matrix $A \in \mathbb{R}^{n \times n}$ is invertible, if and only if all its eigenvalues are nonzero.

Geometry of the eigendecomposition:

$$\text{proj}_v(x) = \frac{x^T v}{\|v\|} v$$



$$Ax = Q \Lambda Q^T x$$

$$\begin{pmatrix} -v_1 \\ -v_2 \end{pmatrix} x = \begin{pmatrix} v_1^T x \\ v_2^T x \end{pmatrix}$$

$$= \begin{pmatrix} c_1 \\ c_2 \end{pmatrix}$$

$$\begin{pmatrix} \tilde{c}_1 \\ \tilde{c}_2 \end{pmatrix} - \begin{pmatrix} \lambda_1 c_1 \\ \lambda_2 c_2 \end{pmatrix} = \begin{pmatrix} 3c_1 \\ c_2 \end{pmatrix}$$

$$Ax = Q \Lambda Q^T x$$

projection

scaling

embedding

$$\left| \begin{array}{ccc} C & \xrightarrow{\Lambda} & \tilde{C} \\ \alpha^T & \uparrow & | \\ X & \longmapsto & Ax \end{array} \right.$$

3.3 Eigenvalue Algorithms: Solving the eigenvalue problem

Aim: Solving the *eigenvalue problem* defined by

Given $A \in \mathbb{F}^{n \times n}$, find eigenpairs (λ_i, v_i) so that, for all $i = 1, \dots, n$,

$$v_i \neq 0 \text{ and } Av_i = \lambda_i v_i.$$

Sometimes we are only interested in a few eigenpairs (λ_i, v_i) (for example the one with largest eigenvalue in magnitude). In this case we call it a *partial* eigenvalue problem.

Overview

1. A first naive approach: Direct method
→ only feasible for very small matrices: $n \in \{2, 3, 4\}$
2. Partial eigenvalue problem: Simple iterative methods (here: The Power Method)
→ determine a *single* eigenpair
3. A second advanced approach: General iterative method (here: The QR algorithm)
→ determine *all* eigenpairs

3.3.1 A first naive approach: Direct method

Recipe:

- a) Eigenvalues:

Solving **root finding problem** for the characteristic polynomial

$$\chi_A(\lambda) := \det(A - \lambda I) = 0$$

yields the eigenvalues λ_i .

- b) Eigenvectors:

Solving the homogeneous **linear system**

$$(A - \lambda_i I)v_i = 0$$

for each distinct λ_i , gives the corresponding eigenvectors v_i (or more precisely, eigenspaces).

Example: $n = 2$

Consider a general (2×2) -matrix $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$.

a) **Root finding problem:**

Above, we have derived a closed formula for the determinant of a (2×2) -matrix, which applied to $A - \lambda I$ gives

$$0 = \chi_A(\lambda) = \det(A - \lambda I) = \det \left(\begin{pmatrix} a - \lambda & b \\ c & d - \lambda \end{pmatrix} \right) = (a - \lambda)(d - \lambda) - cb = \lambda^2 - (a + d)\lambda + (ad - cb)$$

$$\rightarrow \lambda_{1/2} = \frac{a+d}{2} \pm \sqrt{\left(\frac{a+d}{2}\right)^2 - (ad - cb)}.$$

b) **Linear system:**

We then have to solve

$$\begin{pmatrix} a - \lambda_i & b \\ c & d - \lambda_i \end{pmatrix} \begin{pmatrix} v_1^i \\ v_2^i \end{pmatrix} \quad \text{for } i = 1, 2.$$

$$\rightarrow v^1, v^2$$

Note: For $n = 3$ we can proceed similarly by applying the rule of Sarrus in step a).

Problem:

In practice, for general, potentially very large, matrices the root finding problem is infeasible, because:

A with large dimension $n \Rightarrow \chi_A$ high polynomial degree \Rightarrow high risk of rounding errors

See for example:

https://en.wikipedia.org/wiki/Root-finding_algorithms#Roots_of_polynomials

Abel–Ruffini theorem (see related discussion in [4, Theorem 25.1]):

There are no “closed formulas” for the roots of general polynomials with degree higher than 4.

As a consequence:

We cannot solve the eigenvalue problem in finitely many steps.

Instead, any eigenvalue algorithm has to be iterative!

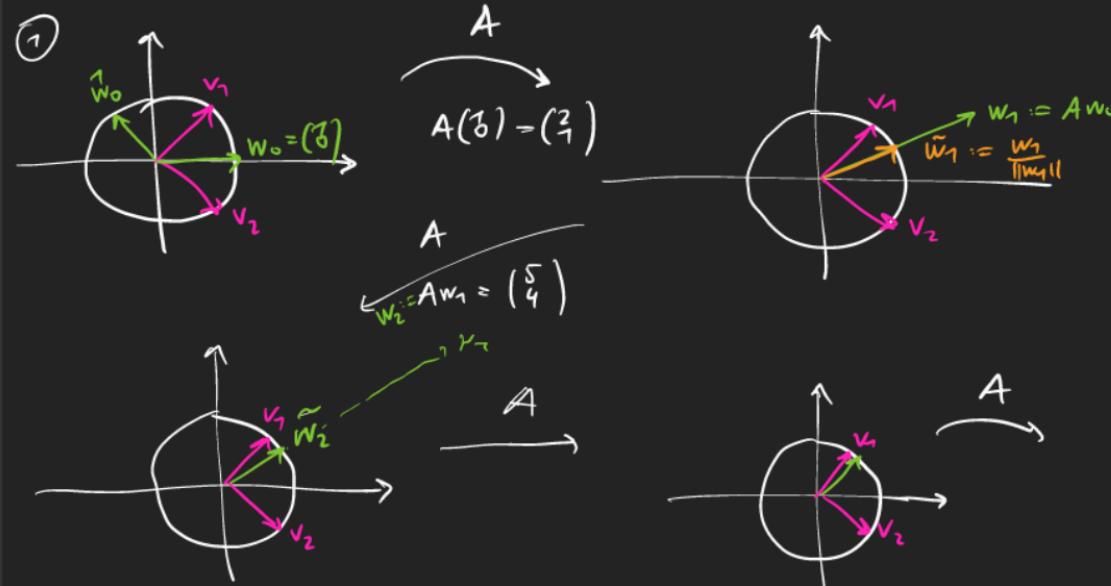
3.3.2 Simple Iterative Method: The Power Iteration

→ basis for PageRank algorithm from Google and the WTF algorithm from Twitter

Example 3.9 (Illustration in 2d: Part 5)

Again, let us consider $A = \begin{pmatrix} 2 & 1 \\ 1 & 2 \end{pmatrix}$, $\lambda_1 = 3$, $v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$, $\lambda_2 = 1$, $v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$.

Let us successively apply the matrix A to an initial guess $w^0 \in \mathbb{R}^n$:



Note: The normalization step can be performed with respect to any norm.

Theorem 3.10 (Convergence of power iteration) Let $A \in \mathbb{R}^{n \times n}$ be a matrix with eigenvalues λ_i for $i \in \{1, \dots, n\}$ which satisfy $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$ and whose eigenvectors form a basis of \mathbb{R}^n . Also, let the sequence of vectors $\{w^k\}_{k=0}^\infty$ be defined by the so-called **power iteration**

$$w^{k+1} := \frac{Aw^k}{\|Aw^k\|_p}, \quad k \geq 0, p \geq 1, \quad \text{with } w^0 \text{ such that } (v^1, w^0)_2 \neq 0,$$

where v^1 is the normalized (i.e., $\|v^1\|_p = 1$) eigenvector corresponding to λ_1 . Then, for $k \rightarrow \infty$, we find $w^k \rightarrow \pm v^1$ and also the so-called Rayleigh quotients

$$\mu_k := \frac{(w^k, Aw^k)_2}{(w^k, w^k)_2} \rightarrow \lambda_1.$$

Proof. See, e.g., [1, Satz 7.3] or [4, Theorem 27.1]. The idea: Let $v^i \in \mathbb{R}^n$ be the corresponding eigenvectors. Then we can write the initial guess as linear combination $w^0 = \sum_{j=1}^n \mu_j v^j (\mu_1 \neq 0)$, so that with $c_k := \frac{1}{\|Aw^k\|_p}$ we find

$$w^k = c_k A^k w^0 = c_k \sum_{j=1}^n \mu_j A^k v^j = c_k \sum_{j=1}^n \mu_j \lambda_j^k v^j = c_k \lambda_1^k \left(\mu_1 v^1 + \sum_{j=2}^n \mu_j \left(\frac{\lambda_j}{\lambda_1} \right)^k v^j \right).$$

The fractions $\left(\frac{\lambda_j}{\lambda_1} \right)^k$ vanish as $k \rightarrow \infty$ and the limit vector is in $\text{span}(v^1)$. Since $\|w^k\|_p = \|v^1\|_p = 1$ the result follows. \square

Remark:

- A variant of this approach is given by the so-called **inverse power method**, which can estimate any eigenpair, assumed a good initial guess for the eigenvalue is available.
- The assumption on the eigenvectors is satisfied, e.g., for real symmetric matrices (see Theorem ??)
- From the proof idea one finds that the convergence speed is determined by the fraction $\left(\frac{\lambda_2}{\lambda_1} \right)^k$ (potentially very slow).

3.3.3 A second advanced approach: General iterative method

Recall: (Lemma ??)

- a) **Similar matrices** have the same eigenvalues:

$$\sigma(A) = \sigma(T^{-1}AT) \quad \text{for } T \in GL_n(\mathbb{F}).$$

- b) **Simple matrices**: Eigenvalues of an upper triangular matrix U (e.g., a diagonal matrix) are found on its diagonal, i.e.,

$$\sigma(U) = \{u_{11}, \dots, u_{nn}\}.$$

Recipe:

- a) Iteratively applying **similarity transformations** $T_k \in GL_n(\mathbb{F})$ to $A =: A_0$ thereby producing a sequence

$$A_k = T_k^{-1}A_{k-1}T_k.$$

- b) Choose T_k so that this sequence converges to a **simple matrix** (triangular or even diagonal)

$$A_\infty := \lim_{k \rightarrow \infty} A_k.$$

→ **Question:** Choice of the T_k 's?

Requirements on the transformations T_k :

1. easily constructed from A_{k-1}
2. easy to invert (e.g., orthogonal matrix)
3. $(A_k)_k$ converges to something simple

One Implementation:

- a) The **QR-Algorithmn** defines such transformations T_k through

$$A_0 = A$$

for $k = 1, \dots, \infty$:

$$Q_k R_k := A_{k-1}$$
$$A_k := R_k Q_k$$

Thus, inserting the first equation $R_k = Q_k^T A_{k-1}$ into the second gives

$$A_k = R_k Q_k = Q_k^T A_{k-1} Q_k = Q_k^T Q_{k-1}^T A_{k-2} Q_{k-1} Q_k = \dots = \overline{Q}_k^T A \overline{Q}_k$$

where

$$\overline{Q}_k := Q_1 \cdot Q_2 \cdots Q_{k-1} \cdot Q_k$$

Here: $T_k = Q_{k-1}$, where Q_{k-1} is derived from the QR decomposition of A_{k-1} .

b) We find: $A_k = \overline{Q}_k^T A \overline{Q}_k \xrightarrow[k \rightarrow \infty]{} U$, where U is **(quasi) upper triangular**; given as follows:

Theorem 3.11 (QR Algorithm) Consider a matrix $A \in \mathbb{R}^{n \times n}$ with distinct eigenvalues λ_i for $i = 1, \dots, n$, i.e., $|\lambda_1| > |\lambda_2| > \dots > |\lambda_n|$. Then the iterates $A_k \in \mathbb{R}^{n \times n}$ produced by the QR algorithm converge to the diagonal matrix $\Lambda := \text{diag}(\lambda_1, \dots, \lambda_n)$ which consists of the eigenvalues of A , i.e.,

$$\lim_{k \rightarrow \infty} A_k = \Lambda.$$

Proof. See, e.g., [1, Satz 7.8]. □

Finally: **What about the eigenvectors?**

One can further show that similar to the power iteration, we find that the columns of

$$\overline{Q}_\infty := \lim_{k \rightarrow \infty} \overline{Q}_k$$

are normalized eigenvectors of A .

3.3.4 In Practice: Combined Iterative Methods

Problems:

- QR decomposition for general and very large matrices too expensive
- Exact Schur complement is not reached in finitely many steps (= many QR decompositions needed)

However:

- Any matrix can be **reduced** to a Hessenberg matrix (= simple matrix) in *finitely many* steps
- QR decomposition for this type of matrix is cheap

This leads to:

(3) A third state-of-the-art approach: Combined iterative methods

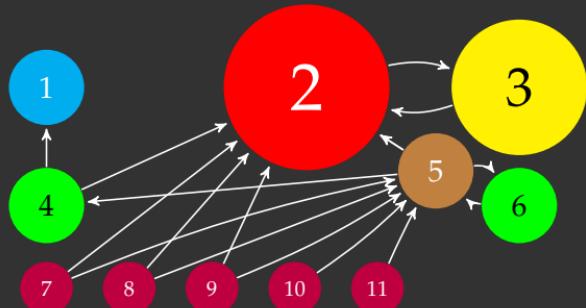
- a) **Similarity transformation via reduction** (e.g., Householder, Wilkinson, Givens) to something simple such as Hessenberg or even tridiagonal
(→ *finite steps*)
- b) **Similarity transformation via iterative method** (e.g., QR or LR algorithm)
(→ *potentially infinitely many steps*)
Standard: QR Algorithm (with performance optimized modifications (shifts etc...))
- c) Determine eigenvalues from the limiting **simple matrix** (and eigenvectors from the similarity transformations).

Common combination in practice: (a) Householder reflection + (b) QR algorithm

→ Works pretty well for matrices up to 1 mio. columns $n \approx 10^6$

→ for larger matrices one needs to develop problem-tailored structure exploiting methods

3.4 Example: The PageRank Algorithm from Google



Aim: Rank search engine results according to the “*importance*” of the web pages.

1998: For this purpose, Larry Page and Sergei Brin develop the PageRank algorithm as the basis of the **Google** empire.

Assumption: “*important*” means more links from other (*important*) web pages.

→ More details on the sheet and in the video.

Singular Value Decomposition (SVD)

Recommended reading:

- Lectures 4, 5 in [4]
- Sections I.8 and I.9 in [3]

Literature:

[1] R. Rannacher.

Numerik 0 - Einführung in die Numerische Mathematik.

Heidelberg University Publishing, 2017.

[2] G. Strang.

Introduction to Linear Algebra.

Wellesley-Cambridge Press, 2003.

[3] G. Strang.

Linear Algebra and Learning from Data.

Wellesley-Cambridge Press, 2019.

[4] L.N. Trefethen and D. Bau.

Numerical linear algebra.

SIAM, Soc. for Industrial and Applied Math., Philadelphia, 1997.

4 Singular Values and the Singular Value Decomposition (SVD)

We will extend the concept of eigenvalues and eigenvectors to general matrices $A \in \mathbb{R}^{m \times n}$.

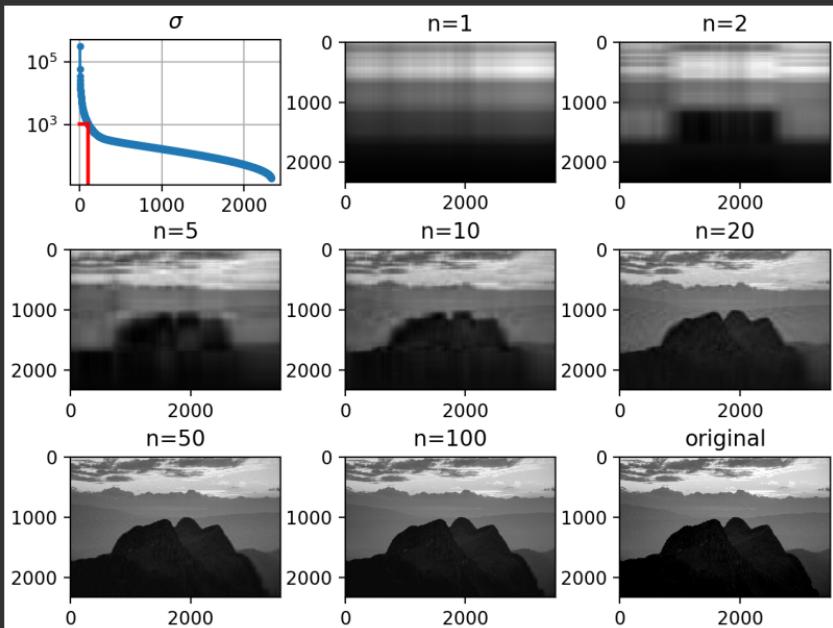
4.1 Motivation and Introduction

Gilbert Strang: “*The SVD $A = U\Sigma V^\top$ is the **most important** theorem in data science.*”
([3] Linear Algebra and Learning from Data, p.31)

Importance and Applications:

- The SVD of a matrix reveals many properties about the matrix itself (representation of the image and kernel, rank, invertibility, condition,...)
- Low-Rank Approximation
 - Data compression (e.g., image data)
 - Principal Component Analysis
- Pseudoinverse (generalization of the inverse matrix) and relation to the minimum-norm least squares solution

Image and data compression:



3500×2333 greyscale image is interpreted as matrix

$$A \in [0, 1]^{3500 \times 2333}.$$

The singular values are shown in the figure with the title " σ ".

The reconstructed image with the first 100 singular values only, i.e.,

$$A_{100} := U \text{diag}(\sigma_1, \dots, \sigma_{100}, 0, \dots, 0) V^\top$$

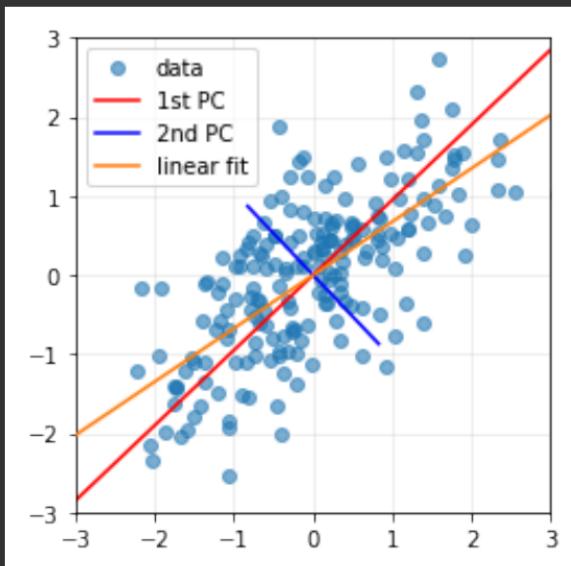
is quite close to the original image but takes only

$$\frac{3500 \cdot 100 + 100 \cdot 100 \cdot 2333}{3500 \cdot 2333} \approx 7\%$$

of the storage space.

Principal Component Analysis

Under the correct setup we have that the SVD equals the PCA, whose aim is dimension reduction:



The data represented by the blue dots can be fully explained by the red and blue line. However the red line might already capture a substantial part of the data's variance.

The Singular Value Decomposition (SVD)

For matrices $A \in \mathbb{R}^{m \times n}$ of general format, the equation $Av = \lambda v$ fails. Instead we define:

Definition 4.1 (Singular Values and Vectors) Let $A \in \mathbb{R}^{m \times n}$ be a matrix. Then a positive number $\sigma > 0$ is called **singular value**, if there exist nonzero vectors $v \in \mathbb{R}^n \setminus \{0\}$ and $u \in \mathbb{R}^m \setminus \{0\}$, such that

$$Av = \sigma u \quad \text{and} \quad A^\top u = \sigma v. \quad (8)$$

The vectors v and u are called right and left **singular vectors of A to the singular value σ** .

Assume we had singular vectors v_i, u_i and values σ_i and put them into matrices V, U, Σ (as we did for the eigendecomposition). Then we find

$$AV = U\Sigma$$

This will lead to the impactful theorem of the singular value decomposition:

Theorem 4.2 (Singular value decomposition (SVD)) Let $A \in \mathbb{R}^{m \times n}$. Then there are orthogonal matrices $U \in \mathbb{R}^{m \times m}$ and $V \in \mathbb{R}^{n \times n}$ as well as a diagonal matrix $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0) \in \mathbb{R}^{m \times n}$, where $\sigma_1 \geq \sigma_2 \geq \dots \geq \sigma_r > 0$, $r \leq \min\{m, n\}$, are the sorted positive singular values, such that

$$A = U\Sigma V^\top,$$

which is the so-called **singular value decomposition of A** .

4.2 Preparing Results

In order to understand and prove this central theorem we will put a few auxiliary results into position. The first one is about eigenvalues of symmetric and positive semi-definite matrices:

Lemma 4.3 (Eigenvalues and Positivity) Let $B \in \mathbb{R}^{n \times n}$ be symmetric and positive definite (semi-definite), then $\lambda > 0$ (≥ 0) for all eigenvalues $\lambda \in \sigma(B)$.

Proof. First of all we note that due to symmetry $\sigma(B) \subset \mathbb{R}$ and we can choose eigenvectors with real coefficients.

We now perform a proof by contradiction:

Let B be positive definite and assume $\lambda \leq 0$ for some $\lambda \in \sigma(B)$ with eigenvector $v \in \mathbb{R}^n, v \neq 0$.
 $\Leftrightarrow x^\top Bx > 0 \quad \forall x \neq 0$ $\Leftrightarrow \exists v \neq 0: Bv = \lambda v$

Then we find

$$v^\top \underbrace{Bv}_{= \lambda v} = \lambda v^\top v = \underbrace{\lambda}_{\leq 0} \underbrace{\|v\|_2^2}_{> 0} \leq 0 \quad [\text{contradiction to the positivity of } A].$$

(Analogous proof for B positive semi-definite.)

(Alternative proof via Rayleigh quotient.)

□

The next result is about the shared eigenvalues of product matrices:

Lemma 4.4 (Shared Eigenvalues of Products) *Let $A \in \mathbb{F}^{m \times n}$ and $B \in \mathbb{F}^{n \times m}$. Then the products $AB \in \mathbb{F}^{m \times m}$ and $BA \in \mathbb{F}^{n \times n}$ have the same nonzero eigenvalues.*

Proof. We prove this by mutual subset relation:

First let $\lambda \in \sigma(AB), \lambda \neq 0$ be a nonzero eigenvalue of AB with eigenvector $v \in \mathbb{F}^n, v \neq 0$, i.e.,

$$ABv = \lambda v.$$

Now multiply both sides by B to obtain

$$BA(Bv) = \lambda Bv,$$

which implies that Bv is an eigenvector of BA with the *same* eigenvalue λ . To see this, note that $\lambda \neq 0$ implies that $ABv = \lambda v \neq 0$ and thus $Bv \neq 0$.

Similarly, let now $\lambda \in \sigma(BA), \lambda \neq 0$ be a nonzero eigenvalue of BA with eigenvector $v \in \mathbb{F}^n, v \neq 0$, i.e., $BAv = \lambda v$. Then we multiply both sides by A to proceed along the same lines. \square

Remark:

- If $m \neq n$, then BA and AB have differently many eigenvalues. However the nonzero eigenvalues are the same. Thus both product matrices have at most $\ell := \min\{m, n\}$ nonzero eigenvalues!
- In the special case that $m = n$ and B invertible, we observe

$$B^{-1}(BA)B = (AB),$$

identifying the matrices AB and BA as being similar!

Now a special instance of the latter two results (choosing $B = A^\top$) leads us to the key lemma to prove the SVD Theorem ??:

Lemma 4.5 Let $A \in \mathbb{R}^{m \times n}$, then the matrices $A^\top A$ and AA^\top are symmetric, positive semi-definite and have the same positive eigenvalues.

Proof. We find:

- 1) Symmetry: $(A^\top A)^\top = A^\top (A^\top)^\top = A^\top A$ and similarly $(AA^\top)^\top = AA^\top$
- 2) p(s)d: $x^\top A^\top Ax = \|Ax\|_2^2 \geq 0$, $x^\top AA^\top x = \|A^\top x\|_2^2 \geq 0$
- 3) The same positive eigenvalues:
 - By Lemma ?? we know that the matrices only have nonnegative eigenvalues
 - By lemma ?? we know that the nonzero, i.e., positive, eigenvalues are the same

□

Remark:

Due to the symmetry of $A^\top A$ and AA^\top we also know that we find orthonormal eigenvectors v_1, \dots, v_n and u_1, \dots, u_m ! The SVD will connect them!

4.3 From Reduced to Full SVD

Recall:

- $\text{Im}(A) \perp \ker(A^\top)$ and $\text{Im}(A^\top) \perp \ker(A)$
- $A^\top A, AA^\top$ are
 - symmetric \Rightarrow real eigenvalues and we find orthonormal basis of eigenvectors
 - positive semi-definite \Rightarrow their eigenvalues are nonnegative, i.e., $\lambda \geq 0$
 - they have the same positive eigenvalues λ_i for $1 \leq i \leq r \leq \min(m, n)$
 - $\ker(A) = \ker(A^\top A)$ and $\ker(A^\top) = \ker(AA^\top)$

Proof of SVD: We are looking for nonzero vectors $u \in \mathbb{R}^m, v \in \mathbb{R}^n$ and positive numbers $\sigma > 0$, such that

$$Av = \sigma u \iff u = \frac{1}{\sigma} Av \in \text{Im}(A), \quad (9)$$

$$A^\top u = \sigma v \iff v = \frac{1}{\sigma} A^\top u \in \text{Im}(A^\top). \quad (10)$$

1) So we have two equations for two unknown vectors. By inserting one into the other we obtain two equivalent formulations (this is *elimination*). Here, we insert (??) into (??) which gives

$$A^\top Av = \sigma^2 v \iff (\sigma^2, v) \text{ eigenpair of } A^\top A. \quad (11)$$

(Note: Inserting (??) into (??) would give (σ^2, u) eigenpair of AA^\top)

2) Let $\lambda_1, \dots, \lambda_r > 0$ ($r \leq \min(m, n)$) be the positive eigenvalues of $A^\top A$ with orthonormal eigenvectors v_1, \dots, v_r ($\in \text{Im}(A^\top)$). Then according to (??) and (??) we set

$$\sigma_i := \sqrt{\lambda_i}, \quad u_i := \frac{1}{\sigma_i} Av_i \quad (\in \text{Im}(A)).$$

We then find:

- By construction v_i, u_i are singular vectors to the singular value σ_i , i.e., we have

$$Av_i = \sigma_i u_i$$

and indeed

$$A^\top u_i = \frac{1}{\sigma_i} \underbrace{A^\top Av_i}_{=\lambda_i v_i} = \frac{\lambda_i}{\sigma_i} v_i = \sigma_i v_i.$$

- For the SVD we want the u_i to be orthonormal. Let us check this:

$$u_i^\top u_j = \frac{1}{\sigma_i} \frac{1}{\sigma_j} (Av_i)^\top A v_j = \frac{1}{\sigma_i} \frac{1}{\sigma_j} v_i^\top \underbrace{A^\top A v_j}_{=\lambda_j v_j} = \underbrace{\frac{\sigma_j}{\sigma_i}}_{=\delta_{ij}} v_i^\top v_j = \delta_{ij}.$$

Full, Reduced and Truncated SVD

$$\begin{aligned}
 A &= \left(\begin{array}{c|ccccc|c} | & & | & & | & & | \\ u_1 & \cdots & u_r & u_{r+1} & \cdots & u_m & | \end{array} \right) \left(\begin{array}{ccc|c} \sigma_1 & & & \vdots \\ & \ddots & & 0 \\ & & \sigma_r & \vdots \\ \hline & \vdots & & \vdots \\ \cdots & 0 & \cdots & 0 & \cdots \\ & & & \vdots & \vdots \end{array} \right) \left(\begin{array}{ccc} - & v_1 & - \\ - & \vdots & - \\ - & v_r & - \\ - & v_{r+1} & - \\ - & \vdots & - \\ - & v_n & - \end{array} \right) \quad (\text{full SVD}) \\
 &= (U_r \Sigma_r \mid 0) \begin{pmatrix} V_r^\top \\ \vdots \\ * \end{pmatrix} \\
 &= U_r \Sigma_r V_r^\top \quad (\text{reduced SVD}) \\
 &= \left(\begin{array}{c|c} | & | \\ \sigma_1 u_1 & \cdots & \sigma_r u_r \\ | & | \end{array} \right) \left(\begin{array}{ccc} - & v_1 & - \\ - & \vdots & - \\ - & v_r & - \end{array} \right) \\
 &= \sum_{j=1}^r \sigma_j u_j v_j^\top = \sigma_1 u_1 v_1^\top + \sigma_2 u_2 v_2^\top + \cdots + \sigma_r u_r v_r^\top \quad (\text{sum of rank-1 matrices}) \\
 &\approx \sigma_1 u_1 v_1^\top + \cdots + \sigma_k u_k v_k^\top \quad (\text{truncated SVD } (k < r))
 \end{aligned}$$

The four fundamental subspaces revisited:

By Lemma ?? (note: $U_r \Sigma_r$ is injective and $\Sigma_r V_r^\top$ is surjective) we find

$$\text{Im}(A) = \text{Im}(U_r \Sigma_r V_r^\top) = \text{Im}(U_r) = \text{span}(u_1, \dots, u_r),$$

$$\ker(A) = \ker(U_r \Sigma_r V_r^\top) = \ker(V_r^\top) = \text{Im}(V_r)^\perp = \text{span}(v_{r+1}, \dots, v_n)$$

and by considering $A^\top = V \Sigma^\top U^\top$ we find

$$\text{Im}(A^\top) = \text{span}(v_1, \dots, v_r),$$

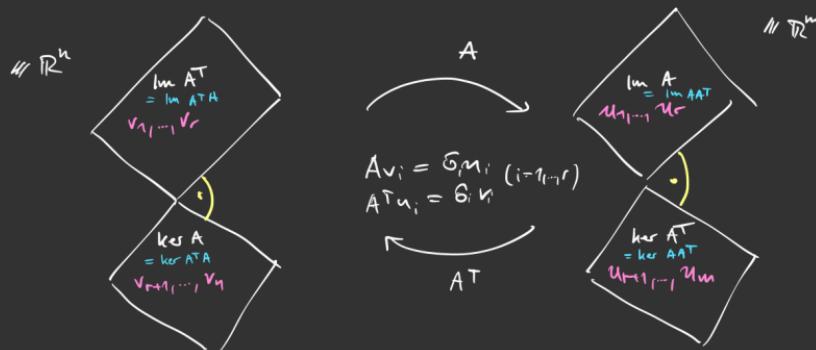
$$\ker(A^\top) = \text{span}(u_{r+1}, \dots, u_m).$$

With other words:

The SVD contains orthonormal bases for all four fundamental subspaces.

And even more than that, they are connected via

$$Av = \sigma u, \quad A^\top u = \sigma v.$$



Summary and Remarks

$$A = \left(\begin{array}{c|cc|cc|c} & & & & & \\ u_1 & \cdots & u_r & u_{r+1} & \cdots & u_m \\ \hline & & & & & \\ & & & & & \\ & & & & & \\ & & & & & \\ \end{array} \right) \left(\begin{array}{ccc|cc|c} \sigma_1 & & & & & \vdots \\ & \ddots & & & & 0 & \cdots \\ & & \sigma_r & & & \vdots \\ \hline & & & & & \vdots \\ \vdots & & & & & 0 & \cdots \\ & 0 & \cdots & & & 0 & \cdots \\ \hline & & & & & \vdots & \\ \vdots & & & & & & \end{array} \right) \left(\begin{array}{ccc} - & v_1 & - \\ \vdots & \vdots & \vdots \\ - & v_r & - \\ - & v_{r+1} & - \\ \vdots & \vdots & \vdots \\ - & v_n & - \end{array} \right)$$

- we can show $\text{Im}(A) = \text{span}(u_1, \dots, u_r)$ and $\ker(A) = \text{span}(v_{r+1}, \dots, v_n)$, in particular

$$\text{rank}(A) = r$$

- columns of V are orthonormal eigenvectors of $A^\top A \in \mathbb{R}^{n \times n}$ and $A^\top A = V(\Sigma^\top \Sigma)V^\top$
- columns of U are orthonormal eigenvectors of $AA^\top \in \mathbb{R}^{m \times m}$ and $AA^\top = U(\Sigma \Sigma^\top)U^\top$
- σ_1^2 to σ_r^2 are the shared positive eigenvalues of both $A^\top A$ and AA^\top
- an SVD of the transpose A^\top is easily found by

$$A^\top = (U\Sigma V^\top)^\top = V\Sigma^\top U^\top$$

- for square matrices singular values and eigenvalues are different in general, take for example $A = -I$
- however, for symmetric matrices $A = Q\Lambda Q^\top$, the singular values are the absolute values of the eigenvalues, i.e., $\sigma_i = \sqrt{\lambda_i^2}$ (see exercises)

Example 4.6 (SVD by hand)

$$A = \begin{bmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{bmatrix}, A^\top = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix}$$

$$A^\top A = \begin{bmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{bmatrix} \begin{bmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{bmatrix} = \begin{bmatrix} 17 & 8 \\ 8 & 17 \end{bmatrix}$$

- Compute eigenvalues of $A^\top A$:

$$0 \stackrel{!}{=} \det(A^\top A - \lambda I) = \det \begin{pmatrix} 17 - \lambda & 8 \\ 8 & 17 - \lambda \end{pmatrix} = (17 - \lambda)^2 - 64$$

$$\Leftrightarrow 17 - \lambda = \pm 8$$

$$\Leftrightarrow \lambda = 17 \pm 8$$

$$\Leftrightarrow \lambda_1 = 25, \lambda_2 = 9$$

- Compute corresponding normalized eigenvectors:

$$\text{a) } (A^\top A - \lambda_1 I)v_1 = \begin{pmatrix} -8 & 8 \\ 8 & -8 \end{pmatrix} v_1 \stackrel{!}{=} 0 \Rightarrow v_1 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$\text{b) } (A^\top A - \lambda_2 I)v_2 = \begin{pmatrix} 8 & 8 \\ 8 & 8 \end{pmatrix} v_2 \stackrel{!}{=} 0 \Rightarrow v_2 = \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

- Compute left singular vectors:

$$\sigma_1 := \sqrt{\lambda_1} = 5,$$

$$u_1 := \frac{1}{\sigma_1} Av_1$$

$$= \frac{1}{5\sqrt{2}} \begin{pmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

$$= \frac{1}{5\sqrt{2}} \begin{pmatrix} 5 \\ 5 \\ 0 \end{pmatrix}$$

$$= \frac{1}{\sqrt{2}} \begin{pmatrix} 1 \\ 1 \\ 0 \end{pmatrix}$$

$$\sigma_2 := \sqrt{\lambda_2} = 3,$$

$$u_2 := \frac{1}{\sigma_2} Av_2$$

$$= \frac{1}{3\sqrt{2}} \begin{pmatrix} 3 & 2 \\ 2 & 3 \\ 2 & -2 \end{pmatrix} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

$$= \frac{1}{3\sqrt{2}} \begin{pmatrix} 1 \\ -1 \\ 4 \end{pmatrix}$$

Find $u_3 \in \ker(A^\top)$:

$$A^\top u_3 = \begin{pmatrix} 3 & 2 & 2 \\ 2 & 3 & -2 \end{pmatrix} \begin{pmatrix} u_3^1 \\ u_3^2 \\ u_3^3 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

$$u_3 = \frac{1}{3} \begin{pmatrix} 2 \\ -2 \\ -1 \end{pmatrix}$$

Example: rank-1 pieces

Let $x \in \mathbb{R}^m \setminus \{0\}$ and $y \in \mathbb{R}^n \setminus \{0\}$, then

$$A := xy^\top = \begin{pmatrix} x_1 \\ \vdots \\ x_m \end{pmatrix} (y_1, \dots, y_n) = \begin{pmatrix} | & & | \\ y_1 x & \cdots & y_n x \\ | & & | \end{pmatrix} \in \mathbb{R}^{m \times n}.$$

What is the SVD of A ?

$$A^\top A = (xy^\top)^\top xy^\top = y \underbrace{x^\top x}_{=\|x\|^2} y^\top = \|x\|^2 yy^\top$$

Compute eigenpairs: We find $A^\top Ay = \|x\|^2 y \underbrace{y^\top y}_{=\|y\|^2} = \|x\|^2 \|y\|^2 y$

$v_1 := \frac{y}{\|y\|}$ is eigenvector to the eigenvalue $\lambda_1 := \|x\|^2 \|y\|^2$

Set

$$\sigma_1 := \sqrt{\lambda_1} \stackrel{(\neq 0, \text{ since } x \neq 0 \neq y)}{=} \|x\| \|y\|$$

and

$$u_1 := \frac{1}{\sigma_1} Av_1 = \frac{1}{\|x\| \|y\|} xy^\top \frac{y}{\|y\|} = \frac{x}{\|x\|}$$

then

$$A = U\Sigma V^\top = \frac{x}{\|x\|} (\|x\| \|y\|) \frac{y^\top}{\|y\|} = xy^\top \checkmark \quad (\rightarrow r = 1, \text{ thus } \text{rank}(A) = 1)$$

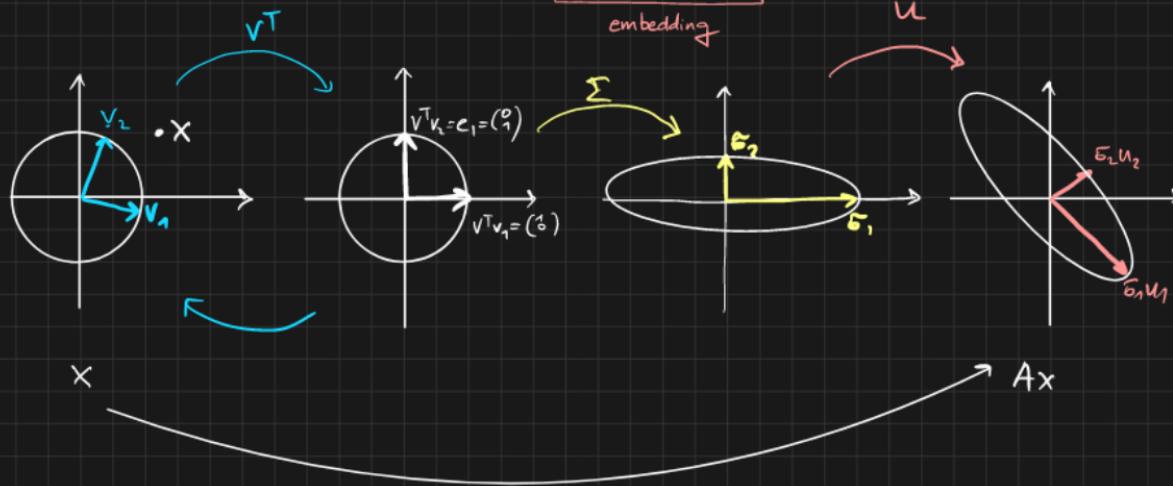
4.4 The Geometry of the SVD

[Compare to the geometry of the eigendecomposition]

- GEOMETRY:

$$A \cdot x = U \cdot \sum \underbrace{\sigma_j v_j^T}_{\text{projection}} \cdot x$$

projection
 scaling
 embedding



$$x = \mu_1 v_1 + \mu_2 v_2$$

$$\Rightarrow A x = \mu_1 \sigma_1 u_1 + \mu_2 \sigma_2 u_2$$

- The orthonormal bases V and U are connected via $Av_j = \sigma_j u_j$.
- Using these orthonormal bases, one can regard *any* matrix as a diagonal matrix.

4.5 Matrix condition and rank

Situation:

Let $A = U\Sigma V^\top \in \mathbb{R}^{n \times n}$ be invertible (i.e., $\sigma_i \neq 0 \ \forall i$) and assume we want to solve $Ax = b$. We also assume that the data is corrupted $\tilde{b} = b + \Delta b$ by some error Δb .

\Rightarrow We obtain a perturbed solution $\tilde{x} = x + \Delta x$ with $\Delta x = A^{-1}\Delta b$.

Question:

How severe is the propagation of *data error* Δb to the resulting *solution error* Δx ?

\rightarrow Singular (eigen-) values give us this information!

$$b = Ax \Rightarrow \|b\|_2 = \|Ax\|_2 = \|U\Sigma V^\top x\|_2 = \|\Sigma V^\top x\|_2 = \|\sum_{j=1}^r \sigma_j v_j^\top x\|_2 \leq \sigma_1 \|V^\top x\|_2 = \sigma_1 \|x\|_2$$

$$\Delta x = A^{-1}\Delta b \Rightarrow \|\Delta x\|_2 = \|A^{-1}\Delta b\|_2 = \|V\Sigma^{-1}U^\top \Delta b\|_2 = \|\Sigma^{-1}U^\top \Delta b\|_2 \leq \frac{1}{\sigma_n} \|\Delta b\|_2$$

$$\Rightarrow \frac{\|\Delta x\|_2}{\|x\|_2} \leq \frac{1}{\sigma_n} \frac{\|\Delta b\|_2}{\|b\|_2} \leq \frac{\sigma_1}{\sigma_n} \frac{\|\Delta b\|_2}{\|b\|_2}$$

Definition 4.7 (Condition number) Let $A \in \mathbb{R}^{n \times n}$ be a matrix. Then we call

$$\text{cond}_2(A) := \frac{\max\{\sigma_i\}}{\min\{\sigma_i\}}$$

the **condition number** of the matrix A .

Special Case: Symmetric Matrices (exercise)

Let $A \in \mathbb{R}^{n \times n}$ be a real symmetric matrix, then

$$\text{cond}_2(A) = \frac{\max\{|\lambda| : \lambda \in \sigma(A)\}}{\min\{|\lambda| : \lambda \in \sigma(A)\}}.$$

Remark:

If some of the singular values are actually zero or close to zero, the condition number is (almost) ∞ . In this case, we cannot trust any numerical solver (for $Ax = b$) in finite precision, as errors in the data b (e.g., also due to rounding errors) may severely propagate to the computed solution x .

We also call such matrices *rank deficient*.

4.6 The Truncated SVD and its Best Approximation Property

Motivation:

Let the singular values be sorted $\sigma_1 \geq \dots \geq \sigma_r > 0$, $r := \text{rank}(A)$, then the reduced SVD reads as

$$A = \sigma_1 u_1 v_1^\top + \sigma_2 u_2 v_2^\top + \dots + \sigma_i u_i v_i^\top + \dots + \sigma_{r-1} u_{r-1} v_{r-1}^\top + \sigma_r u_r v_r^\top$$

If a σ_i is small, then the matrix $u_i v_i^\top$ does not contribute much to A , and similarly for $\sigma_{i+1}, \dots, \sigma_r$.

What about leaving them out?

This gives rise to the following definition:

Definition 4.8 (Truncated SVD) Let $A = U\Sigma V^\top \in \mathbb{R}^{m \times n}$. For $k < r := \text{rank}(A)$ define $\Sigma_k := \text{diag}(\sigma_1, \dots, \sigma_k) \in \mathbb{R}^{k \times k}$, $U_k := [u_1, \dots, u_k] \in \mathbb{R}^{m \times k}$ and $V_k := [v_1, \dots, v_k] \in \mathbb{R}^{n \times k}$. Then

$$A_k := U \text{diag}(\sigma_1, \dots, \sigma_k, 0, \dots, 0) V^\top = U_k \Sigma_k V_k^\top$$

is called **truncated SVD of A** .

We observe that

$$\text{rank}(A_k) = k,$$

which is why A_k is also called **rank- k -approximation of A** .

Question: Leaving out some rank-1 summands, how much do we deviate from the original matrix?

With other words: In which sense does $A_k \in \mathbb{R}^{m \times n}$ approximate $A \in \mathbb{R}^{m \times n}$?

We first need to quantify the distance between matrices, i.e., we need a *norm* for matrices in $\mathbb{R}^{m \times n}$!

Here we consider the so-called Frobenius norm:

If we reshape a matrix $A \in \mathbb{R}^{m \times n}$ into a vector $v \in \mathbb{R}^{m \cdot n}$ (e.g., $v_{[(j-1) \cdot m + i]} := a_{ij}$), then we can use our norms for vectors, e.g.,

$$\|A\|_F := \|v\|_2.$$

This is precisely:

Definition 4.9 (Frobenius norm) For any matrix $A \in \mathbb{R}^{m \times n}$, the **Frobenius norm** is defined as

$$\|A\|_F := \sqrt{\sum_{i=1}^m \sum_{j=1}^n a_{ij}^2}.$$

Exercise:

- One can show that

$$\|A\|_F^2 = \text{tr}(A^\top A),$$

where $\text{tr} :=$ “trace” denotes the sum of the diagonal entries.

- Using this fact, for $A = U\Sigma V^\top$ with $r = \text{rank}(A)$ we also find

$$\|A\|_F^2 = \sum_{i=1}^r \sigma_i^2.$$

Finally, the truncated SVD satisfies a best approximation property:

Theorem 4.10 (Eckart-Young-Mirsky) Let $A \in \mathbb{R}^{m \times n}$ with SVD $A = U\Sigma V^\top$ and let $k \leq \text{rank}(A)$. Then, the truncated SVD A_k is the best approximation in the Frobenius norm among all matrices with rank k , i.e.

$$\|A - A_k\|_F \leq \|A - B\|_F, \quad \forall B \in \mathbb{R}^{m \times n}, \text{rank}(B) = k.$$

In words:

Among all matrices with rank k , the truncated SVD is closest to A .

Proof. We use the so-called Weyl inequality (see (??) below): For matrices $C, D \in \mathbb{R}^{m \times n}$ with decreasingly ordered singular values, we denote by $\sigma_i(C), \sigma_i(C), \sigma_i(C + D)$ the i -th singular value of the respective matrix. Then Weyl's inequality gives us the relation

$$\sigma_{i+\ell-1}(C + D) \leq \sigma_i(C) + \sigma_\ell(D), \quad \text{with } i, \ell, i + \ell - 1 \in \{1, \dots, p\}, \quad p := \min\{m, n\}. \quad (12)$$

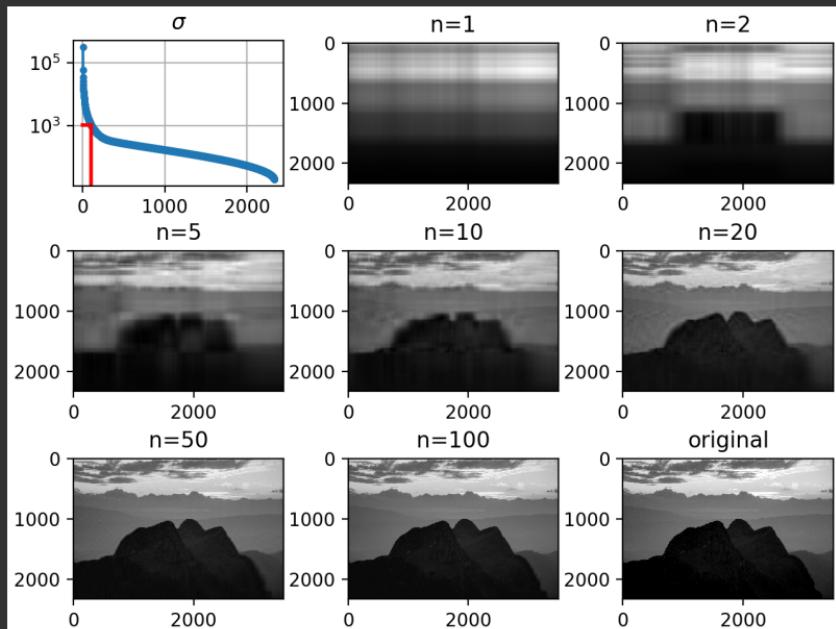
We assume $\text{rank}(B) = k$, which results in $\sigma_l(B) = 0$ for $l > k$ and thus we conclude from Weyl's inequality (??) for $C := A - B, D := B, \ell := k + 1$ that

$$\sigma_{i+k}(A) \leq \sigma_i(A - B) + \sigma_{k+1}(B) = \sigma_i(A - B) \text{ for } i = 1, \dots, p - k$$

$$\Rightarrow \|A - B\|_F^2 = \sum_{i=1}^p \sigma_i(A - B)^2 \geq \sum_{i=1}^{p-k} \sigma_i(A - B)^2 \geq \sum_{i=k+1}^p \sigma_i(A)^2 = \|A - A_k\|_F^2$$

for all B with $\text{rank}(B) = k$. □

4.6.1 Image and Data Compression



Note: The storage of A_k in general is $k \cdot (m + 1 + n)$.

Note: The same data compression can be performed with any matrix — and similarly with tensors.

3500×2333 greyscale image is interpreted as matrix

$$A \in [0, 1]^{3500 \times 2333}.$$

The singular values are shown in the figure with the title “ σ ”.

The reconstructed image with the first 100 singular values only, i.e.,

$$A_{100} := U \text{diag}(\sigma_1, \dots, \sigma_{100}, 0, \dots, 0) V^\top$$

is quite close to the original image but takes only

$$\frac{3500 \cdot 100 + 100 + 100 \cdot 2333}{3500 \cdot 2333} \approx 7\%$$

of the storage space.

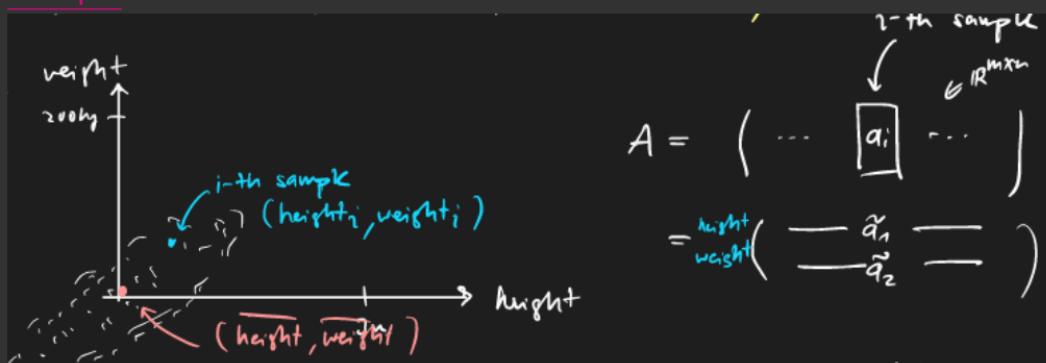
4.6.2 Principal Component Analysis (PCA)

Situation:

n measurements / samples (e.g., questioning n persons)

m features / variables (e.g., height and weight)

Example:



Without loss of generality we can center the data by subtracting the mean from each sample

Observation:

Height and weight are proportional in some sense (i.e., they correlate), however there is some spread/variance.

Aim:

Can we explain "most" of the variance with a lower dimensional subspace?

(In the example above, e.g., a line may capture most of the variance)

Using SVD: $A = U\Sigma V^T$

$$\frac{1}{n-1}AA^T = \frac{1}{n-1}U \begin{pmatrix} \sigma_1^2 & & 0 \\ & \ddots & \\ 0 & & \sigma_r^2 \end{pmatrix} U^T = \frac{1}{n-1} \sum_{i=1}^r \sigma_i^2 u_i u_i^T$$

Thus, the first few summands explain most of AA^T , i.e., the variance

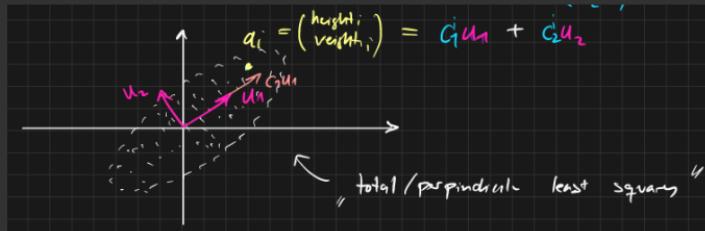
The singular vectors u_1, \dots, u_r are called principal components in this setting.

(Remark: $\|A\|_F = \text{tr}(AA^T) = \sum_{i=1}^m \tilde{a}_i^T \tilde{a}_i = \text{sum of variances}$)

Now to the geometry of the SVD:

$$A = \begin{matrix} m \text{ feats} \\ \downarrow \end{matrix} \quad \xrightarrow{n \text{ samples}} \quad \begin{pmatrix} | & & | & & | \\ a_1 & \cdots & a_i & \cdots & a_n \\ | & & | & & | \end{pmatrix} = U\Sigma V^T = \underbrace{\begin{pmatrix} | & & | \\ u_1 & \cdots & u_m \\ | & & | \end{pmatrix}}_{\substack{\text{orthonormal basis} \\ \text{coordinates of } a_i \text{ in terms of this basis}}} (\underbrace{\Sigma V^T}_{(\Sigma V^T)})$$

Thus, each sample $a_i \in \mathbb{R}^m$ is a linear combination of u_1, \dots, u_m with coefficients $(\Sigma V^T)_i = c_i = \begin{pmatrix} c_1^i \\ c_2^i \end{pmatrix}$



4.6.3 Pseudoinverses

With the help of the SVD one can define a generalized concept of an inverse matrix, called the *pseudoinverse*. This is closely related to the minimum-norm least-squares solution, so that we postpone a discussion to the section on least squares.

4.7 Numerical Computation of the SVD

Let us write equation (??) in matrix form:

$$\begin{pmatrix} 0 & A \\ A^\top & 0 \end{pmatrix} \cdot \begin{pmatrix} u \\ v \end{pmatrix} = \begin{pmatrix} Av \\ A^\top u \end{pmatrix} = \begin{pmatrix} \sigma u \\ \sigma v \end{pmatrix} = \sigma \begin{pmatrix} u \\ v \end{pmatrix}.$$

Then this reads as an eigenvalue problem for the symmetric matrix $S := \begin{pmatrix} 0 & A \\ A^\top & 0 \end{pmatrix}$.

Thus we already identify r eigenpairs for S , namely,

$$(\sigma_1, \begin{pmatrix} u_1 \\ v_1 \end{pmatrix}), \dots, (\sigma_r, \begin{pmatrix} u_r \\ v_r \end{pmatrix}),$$

where $(\sigma_i, \begin{pmatrix} u_i \\ v_i \end{pmatrix})$ are the r singular values and vectors of A , respectively.

Also we easily find that

$$(-\sigma_1, \begin{pmatrix} -u_1 \\ v_2 \end{pmatrix}), \dots, (-\sigma_r, \begin{pmatrix} -u_r \\ v_r \end{pmatrix})$$

are eigenpairs of S .

For the remaining $(m-r)+(n-r)$ eigenpairs take orthonormal bases $u_{r+1}, \dots, u_m \in \ker A^\top$ and $v_{r+1}, \dots, v_n \in \ker A$, then the $(0, \begin{pmatrix} u_i \\ 0 \end{pmatrix})$ and $(0, \begin{pmatrix} 0 \\ v_i \end{pmatrix})$ give the remaining eigenpairs (with eigenvalue 0).

Implications:

→ We can compute the SVD without computing $A^\top A$ or AA^\top .

→ Goes back to Gene Golub in the 1960s (→ see his license plate)

Final Remark:

The SVD is a powerful tool and being able to compute it efficiently further facilitates, among others, the following:

- standard method for computing matrix norms $\|A\|_F$ (or $\|A\|_2 := \sigma_1$)
- the best method for determining the rank of a matrix is to count the number of singular values greater than a judiciously chosen tolerance (note: the fundamental problem is distinguishing a small float which is prone to rounding errors from an actual zero!)
- most accurate method for finding an orthonormal basis of a range or a nullspace
- standards for computing low-rank approximations w.r.t to $\|\cdot\|_F$
- ingredient in robust algorithms for least squares fitting via pseudoinverse

Solving Linear Systems with Iterative Methods

5 Solving Linear Systems with Iterative Methods

5.1 Splitting Methods

Assumption in this section: $A \in \mathbb{R}^{n \times n}$ is invertible, so that $x^* = A^{-1}b$ is the unique solution.

5.1.1 Motivation and Overview

Problem: *The matrix A can be very large ($n \geq 10^5$)!*

- If A can be stored, direct methods (such as LU, QR) are very slow or even not feasible due to large byproducts.
- Often A cannot be stored, so that direct methods are not an option.

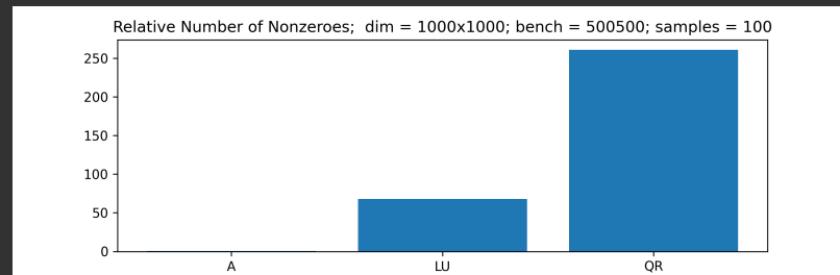
Example:

- A float with double precision (standard) needs 8 bytes of memory.
- Considering 3d measurements with just 100 measurements in each dimension.
 $\Rightarrow 100 \cdot 100 \cdot 100 = 10^6$ measurements
- Discretization methods (e.g., finite element method) for physical models (e.g., heat diffusion) interrelate these measurements.
 \Rightarrow gives a matrix $A \in \mathbb{R}^{n \times n}$ with $n = 10^6$
 $\Rightarrow n \cdot n = 10^{12}$ numbers have to be stored
 $\Rightarrow 10^{12}$ bytes = 1 Terabyte of memory has to be allocated in RAM ↴
- A standard PC nowadays has 8–32 Gbytes of RAM (fast memory).

What if the matrix is *sparse* (= many 0 entries = redundancy)?

- We only need to store nonzero entries and their coordinates (see, e.g., CSR from previous sheets).
- **But:** Direct methods may still produce *dense* (\neq sparse) byproducts.

```
1 A = genRandomSymSparse(D)
2 # NONZEROES OF A
3 nonzeroesA += [np.count_nonzero(A)]
4 # NONZEROS OF LU
5 lu, piv = linalg.lu_factor(A)
6 nonzeroesLU += [np.count_nonzero(lu)]
7 # NONZEROS OF QR
8 Q, R = linalg.qr(A)
9 nonzeroesQR += [(np.count_nonzero(Q)+np.count_nonzero(R))]
10
11 # For sym. matrices we only need to store lower or upper triangle
12 bench = int(D*(D+1)*0.5)
13 # Average
14 nonzeroesA = np.round((np.array(nonzeroesA, dtype=float).sum()/N)/bench*100,2)
15 nonzeroesLU = np.round((np.array(nonzeroesLU, dtype=float).sum()/N)/bench*100,2)
16 nonzeroesQR = np.round((np.array(nonzeroesQR, dtype=float).sum()/N)/bench*100,2)
```



Key idea: We do not need the full matrix, but only some matrix-vector product $x \mapsto S_A x$

Approach: Using this product we define a sequence $\{x^0, x^1, x^2, \dots\} \subset \mathbb{R}^n$ such that

- $x^k \rightarrow x^* \in \mathbb{R}^n$ for $k \rightarrow \infty$
- x^* solves the linear equation $Ax = b$
- x^{k+1} is a better approximation to x^* than x^k

Standard classes of such iterations:

- (1) **Linear iterations (splitting methods)**
- (2) **Krylov subspace methods**

Common advantages:

- Even a few iteration steps may yield good results in stark contrast to LU (Gaussian Elimination), which has to be performed to the bitter end.
 - The matrix A or its decomposition does not need to be stored! Only a **matrix-vector product** $S_A x$ has to be provided.
 - In general, the overall computational complexity is lower than with *direct* methods (LU, QR,...).
- Therefore: Iterative ($=$ *indirect*) methods are to be preferred, when the matrix is large (and sparse).

C.F. Gauß in a letter to Gerling from 1823

(<https://gdz.sub.uni-goettingen.de/id/PPN23601515X?ify>)

Fast jeden Abend mache ich eine neue Auflage des Tableaus, wo immer leicht nachzuhelfen ist. Bei der Einförmigkeit des Messungsgeschäfts gibt dies immer eine angenehme Unterhaltung; man sieht dann auch immer gleich, ob etwas zweifelhaftes eingeschlichen ist, was noch wünschenswerth bleibt, etc. Ich empfehle Ihnen diesen Modus zur Nachahmung. Schwerlich werden Sie je wieder direct eliminiren, wenigstens nicht, wenn Sie mehr als 2 Unbekannte haben. Das indirecte Verfahren lässt sich halb im Schlaf ausführen, oder man kann während desselben an andere Dinge denken.

.....



- He already mentions an iterative method which was later coined *Gauß-Seidel method*.
- In general, one may need a lot of iteration steps but the aim is to keep the iteration instruction simple and fast.

5.1.2 A General Framework: Linear Fixed Point Iteration

Linear iterations are of the form

$$x^{k+1} = Mx^k + Nb$$

with $M, N \in \mathbb{R}^{n \times n}$. The matrix M is called the **iteration matrix** and motivates the adjective “linear”.

We first derive a general convergence result and then relate M and N to the system $Ax = b$.

Convergence analysis

Definition 5.1 (Spectral radius) Let $M \in \mathbb{R}^{n \times n}$. Then the largest eigenvalue of M in magnitude is called the **spectral radius of M** and denoted by $\rho(M)$, more precisely

$$\rho(M) := \max\{|\lambda_1|, \dots, |\lambda_n|\}.$$

Theorem 5.2 (Fixed point iteration) Let $M, N \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$. If $\rho(M) < 1$, then the sequence

$$x^{k+1} = Mx^k + Nb$$

converges for any starting point x^0 and its limit $x^* \in \mathbb{R}^n$ is a fixed point of the affine linear function $x \mapsto Mx + Nb$, i.e.,

$$x^* = Mx^* + Nb.$$

Proof for the special case that M is symmetric:

Let us consider the eigenvalues of M

$$|\lambda_n| \leq |\lambda_{n-1}| \leq \cdots \leq |\lambda_1| =: \rho(M) < 1.$$

Since M is assumed to be symmetric, we can apply the theorem on the eigendecomposition of symmetric matrices and find $Q \in \mathbb{R}^{n \times n}$ orthogonal, $\Lambda \in \mathbb{R}^{n \times n}$ diagonal, so that

$$M = Q\Lambda Q^T, \text{ where } \Lambda = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_n \end{pmatrix}.$$

We will exploit two properties that we can conclude from $\rho(M) < 1$. First, we observe that the powers of M vanish. More precisely,

$$M^2 = M \cdot M = Q\Lambda \underbrace{Q^T Q}_{=I} \Lambda Q^T = Q\Lambda^2 Q^T$$

⋮

$$M^k = Q\Lambda^k Q^T = Q \begin{pmatrix} \lambda_1^k & & 0 \\ & \ddots & \\ 0 & & \lambda_n^k \end{pmatrix} Q^T \xrightarrow[k \rightarrow \infty]{(\rho(M) < 1)} 0.$$

Secondly, we note that the so-called Neumann series converges: $\sum_{j=0}^{\infty} M^j = (I - M)^{-1}$ (general result, no proof here).

Now we are in the position to proof the convergence result. Therefore let $x^0 \in \mathbb{R}^n$, then

$$\begin{aligned} x^{k+1} &= M \cdot \underbrace{x^k}_{= Mx^{k-1} + Nb} + Nb = \underbrace{M^k x^0}_{\xrightarrow{k \rightarrow \infty} 0} + \underbrace{\left(\sum_{j=0}^{k-1} M^j \right)}_{\xrightarrow{k \rightarrow \infty} (I - M)^{-1}} \cdot Nb \xrightarrow{k \rightarrow \infty} (I - M)^{-1} Nb =: x^* \Leftrightarrow Nb = (I - M)x^* \end{aligned}$$

Which is equivalent to $x^* = Mx^* + Nb$. Thus, the limit x^* is a fixed point.

5.1.3 Splitting Methods

We now apply Theorem ?? to the linear system $Ax = b$ by reformulating it as a fixed point problem. We also explain the idea of *preconditioning*.

General scheme:

$$x^{k+1} = Mx^k + Nb$$

First Approach

We rewrite the original system into a fixed point problem:

$$Ax = b \Leftrightarrow (x - x) + Ax = b \Leftrightarrow x = (I - A)x + Ib.$$

Then, if $\rho(I - A) < 1$, we can conclude by Theorem ?? that the fixed point iteration converges

$$x^{k+1} = (I - A)x^k + b \xrightarrow{k \rightarrow \infty} x^*, \text{ with } Ax^* = b.$$

Preconditioning

We see that the success of this procedure relies on the condition $\rho(I - A) < 1$. Unfortunately this is not generally the case, even not for invertible matrices (e.g., $A = 2I \in \mathrm{GL}_n(\mathbb{R})$, then $\rho(I - A) = 1$). An idea to increase our chances is to first *precondition* the original system: Let $N \in \mathbb{R}^{n \times n}$ be invertible, then

$$Ax = b \Leftrightarrow \underbrace{NA}_{=: \tilde{A}} \underbrace{x}_{=: \tilde{b}} = \underbrace{Nb}_{=: \tilde{b}} \Leftrightarrow \tilde{A}x = \tilde{b} \Leftrightarrow x = (I - \tilde{A})x^k + \tilde{b} = (I - NA)x + Nb.$$

Now for this preconditioned fixed point problem: If $\rho(I - NA) < 1$, we can conclude by Theorem ?? that the fixed point iteration converges

$$x^{k+1} = (I - NA)x^k + Nb \xrightarrow{k \rightarrow \infty} x^*, \text{ with } Ax^* = b.$$

What is a good preconditioner?

The optimal choice would be $N = A^{-1}$, because in this case we obtain the solution after one step:

$$x^1 = (I - NA)x^0 + Nb = A^{-1}b.$$

Access to the inverse would make our whole endeavor in this section dispensable. However, it serves as a compass to construct good preconditioners, which are mappings $x \mapsto Nx$ for which $N \approx A^{-1}$.

The advantage and aim of preconditioners are not only to higher our chances for convergence, but also to accelerate the convergence. In fact, by using a good preconditioner $N \approx A^{-1}$, we cannot only make sure that the convergence criteria

$$\rho(I - \tilde{A}) = \rho(I - NA) \ll 1$$

is satisfied, but we can also show that the smaller $\rho(I - NA)$, the faster is the convergence.

How to construct a preconditioner?

- Very simple preconditioning: “Relaxation”

Often it already suffices to make the steps small enough. This idea corresponds to the preconditioner

$$N := \theta I, \text{ with sufficiently small } 0 < \theta \begin{cases} = 1 : & \text{no relaxation} \\ < 1 : & \text{relaxation} \\ > 1 : & \text{over-relaxation} \end{cases}$$

The iteration matrix is then given by

$$M = I - \theta A.$$

- Next idea: “Splitting based”

Recall that the best preconditioner is $N = A^{-1}$, which is not accessible. However, what about inverting just a (significant) part of A ? In order to find such parts which are easy to invert, we consider the splitting of the matrix in the form:

$$\begin{aligned} A &= \begin{pmatrix} \text{yellow} & \text{green} & \text{purple} \\ \text{green} & \text{yellow} & \text{green} \\ \text{purple} & \text{green} & \text{yellow} \end{pmatrix} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} \\ &= L + D + U \end{aligned}$$

For example, D and $(L + D)$ are diagonal and lower triangular, respectively. Thus they are easy to invert (i.e., to solve for) and we may obtain $A^{-1} \approx D^{-1}$ or $A^{-1} \approx (L + D)^{-1}$, respectively.

General scheme:

$$x^{k+1} = (I - NA)x^k + Nb = x^k - N(Ax^k - b)$$

Preconditioner	Iteration Matrix	Iteration Instruction	Method Name
N	$M = I - NA$	$x^{k+1} = x^k - N(Ax^k - b)$	
θI	$M_{Rich} = I - \theta A$	$x^{k+1} = x^k - \theta(Ax^k - b)$	(relax.) Richardson
θD^{-1}	$M_{Jac} = I - \theta D^{-1}A$ $= (1 - \theta)I - \theta D^{-1}(L + U)$	$x^{k+1} = x^k - \theta D^{-1}(Ax^k - b)$ <i>Element-based:</i> $x_i^{k+1} = (1 - \theta)x_i^k + \frac{\theta}{a_{ii}} \left(b_i - \sum_{j \neq i} a_{ij} x_j^{k+1} \right)$	(weighted) Jacobi
$(L + D)^{-1}$	$M_{GS} = I - (L + D)^{-1}A$ $= (L + D)^{-1}U$	$x^{k+1} = x^k - (L + D)^{-1}(Ax^k - b)$ <i>Element-based:</i> $x_i^{k+1} = \frac{1}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{k+1} - \sum_{j=i+1}^n a_{ij} x_j^k \right)$	Gauß-Seidel
$\theta(\theta L + D)^{-1}$	$M_{SOR} = I - \theta(\theta L + D)^{-1}A$ $= (\theta L + D)^{-1}((1 - \theta)D - \theta U)$	$x^{k+1} = x^k - \theta(\theta L + D)^{-1}(Ax^k - b)$ <i>Element-based:</i> $x_i^{k+1} = (1 - \theta)x_i^k + \frac{\theta}{a_{ii}} \left(b_i - \sum_{j=1}^{i-1} a_{ij} x_j^{k+1} - \sum_{j=i+1}^n a_{ij} x_j^k \right)$	Successive Over-Relaxation (SOR)

When does $\rho(M) < 1$ hold?

Idea: Derive some (possibly easy-to-compute) conditions which are sufficient for $\rho(M) < 1$
 → As usual, we often need to assume some properties for A (e.g., symmetry).

Method	Condition
(relax.) Richardson $M_{Rich} = I - \theta A$	<p>With relaxation ($\theta \neq 1$):</p> <p>If A is symmetric and positive definite (spd), then:</p> $\rho(M_{Rich}) < 1 \Leftrightarrow 0 < \theta < \frac{2}{\lambda_{max}(A)}$
(weighted) Jacobi $M_{Jac} = I - \theta D^{-1}A$	<p>No relaxation ($\theta = 1$):</p> <p>If A is strictly diagonally dominant (i.e., $a_{ii} > \sum_{i \neq j} a_{ij}$), then $\rho(M_{Jac}) < 1$</p> <p>With relaxation ($\theta \neq 1$):</p> <p>If A is spd, then:</p> $\rho(M_{Jac}) < 1 \Leftrightarrow 0 < \theta < \frac{2}{\lambda_{max}(D^{-1}A)}$
Gauß-Seidel $M_{GS} = I - (L + D)^{-1}A$	<ul style="list-style-type: none"> • If A is strictly diagonally dominant, then $\rho(M_{GS}) < 1$ • If A is spd, then $\rho(M_{GS}) < 1$
Successive Over-Relaxation (SOR) $M_{SOR} = I - \theta(\theta L + D)^{-1}A$	If A is spd, then $\rho(M_{SOR}) < 1$ for $0 < \theta < 2$

Remark: For many matrix classes (e.g., symmetric), we find

$$\rho(M_{GS}) \leq \rho(M_{Jac}) \leq \rho(M_{Rich}) \quad (\theta = 1).$$

Example

Let us consider the symmetric tridiagonal matrix

$$A = \begin{pmatrix} 3 & -1 & & 0 \\ -1 & \ddots & \ddots & \\ & \ddots & \ddots & -1 \\ 0 & & -1 & 3 \end{pmatrix} = \begin{pmatrix} 0 & & & 0 \\ -1 & \ddots & & \\ & \ddots & \ddots & \\ 0 & & -1 & 0 \end{pmatrix} + \begin{pmatrix} 3 & & & 0 \\ & \ddots & & \\ & & \ddots & 3 \\ 0 & & & 0 \end{pmatrix} + \begin{pmatrix} 0 & -1 & & 0 \\ & \ddots & \ddots & \\ & & \ddots & \\ 0 & & & -1 \end{pmatrix}$$
$$= L + D + U$$

For large n this matrix is extremely sparse:

$$\frac{\#\text{ nonzero entries}}{n^2} = \frac{n+2(n-1)}{n^2} \xrightarrow{n \rightarrow \infty} 0.$$

Based on the convergence criteria from the table above, we now check which methods would converge here. Since $|3| > |-1| + |-1|$ it is easily verified that A is strictly diagonally dominant. Therefore Jacobi and Gauß-Seidel converge.

What about the Richardson method? For simplicity we consider $n = 3$ and compute the eigenvalues of A and find

$$\det(A - \lambda I) = \det \begin{pmatrix} 3 - \lambda & -1 & 0 \\ -1 & 3 - \lambda & -1 \\ 0 & -1 & 3 - \lambda \end{pmatrix}$$
$$\stackrel{\text{Sarrus}}{=} -(3 - \lambda)^3 + (3 - \lambda) + (3 - \lambda)$$
$$= (3 - \lambda) \cdot (2 - (3 - \lambda)^2) \stackrel{!}{=} 0 \Leftrightarrow \lambda = 3, (3 - \lambda) = \pm\sqrt{2} \Leftrightarrow \lambda = 3, \lambda = 3 \pm \sqrt{2}$$

Since all eigenvalues of this symmetric matrix are positive, we have that A is positive definite. Noting that $\lambda_{\max}(A) = 3 + \sqrt{2}$, we apply the above convergence criteria and find that the relaxed Richardson method converges, if the relaxation parameter is chosen from the interval

$$0 < \theta < \frac{2}{\lambda_{\max}(A)} = \frac{2}{3 + \sqrt{2}} \approx 0.45 < 1.$$

Final Remarks

- Using the Richardson iteration we only need the evaluation of the matrix vector product $x \mapsto Ax$ to solve the system $Ax = b$.
- All iterations of the form $x^{k+1} = x^k - N(Ax^k - b)$ can be seen as preconditioned Richardson iterations. Next semester you will learn a strong correspondence between the Richardson method and the gradient method, as well as preconditioned Richardson method and Newton-type methods to minimize functions of the form $f(x) := \frac{1}{2}x^\top Ax - b^\top x$.
- By looking at the element-wise formulas for the Jacobi (with $\theta = 1$) and Gauß-Seidel method (see the orange formulas in the table above) we can understand these methods as alternating methods. Consider for example the simple case $n = 2$ and write out these formulas. Then you will see that we alternately compute the components x_1 and x_2 .
- Similar to a block LU factorization, we can consider blocks A_{ij} (= matrices) instead of numbers a_{ij} in the element-wise formulas of Jacobi and Gauß-Seidel. Thereby, one obtains the block Jacobi and block Gauß-Seidel method. These are highly related to so called additive and multiplicative Schwarz methods, respectively.
- In practice, splitting methods (or more precisely the preconditioner N) are mainly used as preconditioners for Krylov subspace methods, which we will address in the next section.

5.2 Krylov Subspace Methods

5.2.1 Krylov Subspaces

Situation:

- $A \in GL_n(\mathbb{R})$ (invertible, n typically large, but A sparse)
- $b \in \mathbb{R}^n$

We want to solve $Ax = b$, but we cannot work with the matrix as a (dense) “array”. Instead we only have access to the mapping

$$x \mapsto Ax \quad (\text{matrix-vector product}).$$

Then given $b \in \mathbb{R}^n$, we can produce the vectors

$$b, Ab, A^2b, \dots, A^k b.$$

There is not much more to consider. Let us collect all linear combinations of these vectors and give it a name:

Definition 5.3 (Krylov* subspaces) *Let $A \in \mathbb{R}^{n \times n}$ and $b \in \mathbb{R}^n$, then the set*

$$K_r(A, b) := \text{span}\{b, Ab, A^2b, \dots, A^{r-1}b\}$$

is called Krylov Subspace of order $r \geq 1$ generated by A and b .

In order to develop an iterative scheme based on this definition, we look deeper into the Krylov subspaces and first collect some insightful observations.

* named after the Russian engineer Alexei Krylov who developed the idea in a paper published around 1931.

Remarks

i) If $b = 0$, then $A^k b = 0$ for all $A \in \mathbb{R}^{n \times n}$ and all $k \in \mathbb{N}$, so that

$$K_r(A, 0) = \{0\} \quad \forall A \in \mathbb{R}^{n \times n}, r \geq 1.$$

ii) If $b \neq 0$ and $A = I$, then $A^k b = b$ for all $k \in \mathbb{N}$, so that

$$K_r(I, b) = \text{span}\{b\} \quad \forall b \neq 0, r \geq 1.$$

iii) If b is an eigenvector of A to the eigenvalue $\lambda \in \sigma(A)$, then $A^k b = \lambda^k b$, so that $A^k b$ and b are linearly dependent, implying

$$K_r(A, b) = \text{span}\{b\} \quad \forall \text{ eigenvectors } b \text{ of } A.$$

iv) Insight from the power method:

Recall: Let $|\lambda_1| > |\lambda_2| \geq \dots \geq |\lambda_n|$ and $b^T v_1 \neq 0$, then $\frac{A^k b}{\|A^k b\|} \rightarrow v_1$.

Thus, for large k we have that the $A^k b$ point into a “similar direction” – more precisely, into the direction of v_1 . With other words the $A^k b$ become more and more linearly dependent.

v) Dimension of Krylov subspaces:

- Since $(K_r(A, b)) \subset \mathbb{R}^n$ is spanned by r vectors, we clearly have $\dim(K_r(A, b)) \leq \min(r, n)$.
- For $A \in GL_n(\mathbb{R})$ one can show that

$$b, Ab, \dots, A^{r-1}b \text{ are independent} \quad \forall r \leq r_{\max},$$

where r_{\max} is the maximal dimension a Krylov subspace generated by A and b can have, i.e.,
 $r_{\max} := \max_{s \leq n} (\dim K_s(A, b))$.

vi) Next we state the crucial result, which forms the basis for the development of Krylov subspace methods:

Lemma 5.4 *Let $A \in GL_n(\mathbb{R})$ and $b \in \mathbb{R}^n$, then there exists an order $r \leq n$ so that for the solution x^* of $Ax = b$ we have*

$$x^* = A^{-1}b \in K_r(A, b).$$

In particular, we find coefficients $\beta_0, \dots, \beta_{r-1}$, such that

$$x^* = \sum_{j=0}^{r-1} \beta_j A^j b.$$

Proof. Consider the $(n+1)$ vectors $b, Ab, \dots, A^{n-1}b, A^n b$, which are necessarily dependent in \mathbb{R}^n . Thus due to the dependence we find $\alpha_0, \alpha_1, \dots, \alpha_n \in \mathbb{R}$, which are not all zero, so that

$$\begin{aligned} 0 &= \sum_{j=0}^n \alpha_j A^j b = \alpha_0 A^0 b + \alpha_1 A^1 b + \cdots + \alpha_n A^n b \\ &\stackrel{(k:=\text{smallest index with } \alpha_k \neq 0)}{=} \underbrace{\alpha_k}_{\neq 0} A^k b + \alpha_{k+1} A^{k+1} b + \cdots + \alpha_n A^n b \\ &\stackrel{(A^{-(k+1)}.|)}{\Leftrightarrow} 0 = \alpha_k \underbrace{A^{-1} b}_{=x^*} + \alpha_{k+1} A^0 b + \cdots + \alpha_n A^{n-k-1} b \\ &\stackrel{(\alpha_k \neq 0)}{\Leftrightarrow} x^* = \frac{\alpha_{k+1}}{-\alpha_k} A^0 b + \frac{\alpha_{k+2}}{-\alpha_k} A^1 b + \cdots + \frac{\alpha_n}{-\alpha_k} A^{n-k-1} b = \sum_{j=0}^{r-1} \beta_j A^j b, \end{aligned}$$

with $\beta_j := \frac{\alpha_{k+1+j}}{-\alpha_k}$ and $r := n - k$. □

Idea of Krylov Subspace Methods

- In words, the latter lemma states that the sought-after solution can be found in a Krylov subspace of some order $r \leq n$. However we neither generally know r nor the linear coefficients β_j .
- This fact leads to the following general iterative scheme of so-called Krylov subspace methods:
In each iteration step $1 \leq r \leq n$, minimize the residual $\|Ax - b\|_2$ over all $x \in K_r(A, b)$, i.e.,

$$x_r := \underset{x \in K_r(A, b) \subset \mathbb{R}^n}{\operatorname{argmin}} \|Ax - b\|_2^2.$$

Thereby we generate a sequence x_1, x_2, \dots, x_n .

- Since $r \leq n$, we know that in exact arithmetic (neglecting presence of rounding errors) at latest the step $r = n$ (x_n) gives us the exact solution, so that one may call these methods “direct”. However n is typically very large ($\geq 10^5$) and in many examples it turns out that a few steps may already give very good approximations.
- Such methods to solve $Ax = b$ have been developed in the early 1950s; the most famous are:
 - **Conjugate Gradient (CG)** (Hestenes, Stiefel; 1952)
for A symmetric and positive definite
 - **MINimal RESidual (MINRES)** (Paige, Saunders; 1975)
for A symmetric and invertible
 - **General Minimal RESidual (GMRES)** (Schultz, Saad; 1986)
for $A \in GL_n(\mathbb{R})$

→ In this chapter we will derive the GMRES method.

Comparison to other methods

Least squares	Krylov subspace	Splitting
$\hat{x} := \underset{x \in \mathbb{R}^n}{\operatorname{argmin}} \ Ax - b\ _2^2$ $A\hat{x} = \underset{w \in \operatorname{Im}(A)}{\operatorname{argmin}} \ w - b\ _2^2$	$x_r := \underset{x \in K_r(A, b)}{\operatorname{argmin}} \ Ax - b\ _2^2$ $Ax_r = \underset{w \in AK_r(A, b)}{\operatorname{argmin}} \ w - b\ _2^2$	$x_r := Mx_{r-1} + Nb$
\rightsquigarrow Projection of b onto $\operatorname{Im}(A) = A\mathbb{R}^n = \mathbb{R}^n$	\rightsquigarrow Projection of b onto $AK_r(A, b) = \operatorname{span}\{Ab, A^2b, \dots, A^rb\}$ $\subseteq K_{r+1}(A, b)$	
Yields exact solution, i.e., $\hat{x} = A^{-1}b$	In theory: Yields a finite sequence with $x_n = A^{-1}b$	Typically yields an infinite sequence with $x^r \xrightarrow{(k \rightarrow \infty)} A^{-1}b$

As a preparation for what follows, we will first derive an iterative method to find orthonormal bases for Krylov subspaces:

5.2.2 The Arnoldi Iteration

- **Situation:** Let us consider the r -th Krylov subspace

$$K_r(A, b) = \text{span}\{A^0b, A^1b, \dots, A^{r-1}b\}$$

with $r \leq r_{\max} = \max_{s \leq n} (\dim(K_s(A, b)))$, so that all $A^{j-1}b$ are independent and $\dim(K_r(A, b)) = r$.

- **Aim:** Find an orthonormal basis $\{q_1, \dots, q_r\}$ of $K_r(A, b)$.
- **Idea:** Apply the Gram–Schmidt orthogonalization process to the linearly independent vectors $c_j := A^{j-1}b$, $1 \leq j \leq r$.
- **Recall Gram–Schmidt:** Let $c_1, \dots, c_r \in \mathbb{R}^n$, where $r \leq n$, be linearly independent vectors. Then an orthonormal basis $\{q_1, \dots, q_r\}$ of $\text{span}(c_1, \dots, c_r) = \text{Im}(C)$ can be found by the following iterative scheme:

$$q_1 := \frac{c_1}{\|c_1\|}$$

“subtracting projections:” $\hat{q}_j := c_j - \sum_{\ell=1}^{j-1} q_\ell^\top c_j \cdot q_\ell$, $r_{\ell j} := q_\ell^\top c_j$

“normalization:” $q_j := \frac{\hat{q}_j}{\|\hat{q}_j\|_2}$, $r_{jj} := \|\hat{q}_j\|_2$

The matrix perspective: Putting the vectors q_j and r_j (which are computed step by step) into matrices, say Q and R , then we obtain the (reduced) QR-decomposition of C , i.e., a matrix $Q = [q_1, \dots, q_r] \in \mathbb{R}^{n \times r}$ with orthonormal columns and an upper triangular matrix $R \in \mathbb{R}^{r \times r}$ with $r_{ii} \neq 0$, so that $C = QR$, which implies (also see Lemma ??) $\text{Im}(C) = \text{Im}(QR) = \text{Im}(Q) = \text{span}(q_1, \dots, q_r)$.

Now we consider the specific choice $c_j := A^{j-1}b$. By inserting these c_j into the above scheme, we obtain the so called **Arnoldi iteration**:

$$q_1 := \frac{b}{\|b\|_2} \quad (\rightarrow \text{ orthonormal basis for } K_1(A, b) = \text{span}(b), b \neq 0)$$

for $j = 2, \dots, r$:

"subtracting projections:" $\hat{q}_j := Aq_{j-1} - \sum_{\ell=1}^{j-1} q_\ell^\top (Aq_{j-1}) \cdot q_\ell, \quad h_{\ell,j-1} := q_\ell^\top (Aq_{j-1}) \quad (*)$

"normalization:" $q_j := \frac{\hat{q}_j}{\|\hat{q}_j\|_2}, \quad h_{j,j-1} := \|\hat{q}_j\| \quad (**)$

All in all, the Arnoldi process yields an orthonormal basis for $K_r(A, b)$, so that

$$K_r(A, b) = \text{span}(b, Ab, \dots, A^{r-1}b) = \text{span}(q_1, \dots, q_r)$$

or with $Q_r := [q_1, \dots, q_r] \in \mathbb{R}^{n \times r}$ in matrix form

$$K_r(A, b) = \text{Im}(Q_r).$$

Remarks:

- Rearranging $(*)$ and $(**)$ easily gives

$$Aq_{j-1} = \|\hat{q}_j\|_2 \cdot q_j + \sum_{\ell=1}^{j-1} q_\ell^\top (Aq_{j-1}) \cdot q_\ell = \sum_{\ell=1}^j h_{\ell,j-1} q_\ell.$$

With other words, Aq_{j-1} is a linear combination of q_1, \dots, q_j .

- Also observe for $j \leq r$: The first q_1, \dots, q_{j-1} are a basis for $K_{j-1}(A, b)$. Thus, assumed these are given, then in order to find an orthonormal basis for $K_j(A, b)$ we just need to compute one more vector, namely q_j .

5.2.3 GMRES

(with Arnoldi and $x_0 = 0$)

Let us recall the general idea of Krylov subspace methods: In each iteration step we compute

$$x_r := \underset{x \in K_r(A, b)}{\operatorname{argmin}} \|Ax - b\|_2^2.$$

Now we approach this minimization problem in a specific procedure resulting in the GMRES method:

We first find an orthonormal basis $\{q_1, \dots, q_r\}$ of $K_r(A, b)$ so that $K_r(A, b) = \operatorname{span}(q_1, \dots, q_r) = \operatorname{Im}(Q_r)$, where $Q_r := [q_1, \dots, q_r] \in \mathbb{R}^{n \times r}$. Then, since by definition $x_r \in K_r(A, b)$, the minimization problem can be rephrased as

$$x_r = \underset{x \in \operatorname{Im}(Q_r)}{\operatorname{argmin}} \|Ax - b\|_2^2 \stackrel{(x_r = Q_r c_r)}{=} Q_r \cdot \underbrace{\left(\underset{c \in \mathbb{R}^r}{\operatorname{argmin}} \|\textcolor{brown}{A}Q_r c - b\|_2^2 \right)}_{=: c_r, \text{ standard least squares problem}}.$$

The least squares problem can then be solved with the help of the QR-decomposition of the design matrix $\textcolor{brown}{A}Q_r$, say $\tilde{Q}_r \tilde{R}_r := \textcolor{brown}{A}Q_r$, so that the corresponding normal equation reads as

$$\tilde{R}_r c_r = \tilde{Q}_r^T b \quad (\text{when is } \tilde{R}_r \text{ invertible?})$$

Thus, GMRES boils down to the three steps. For $1 \leq r \leq n$, do

- Step 1: Find an orthonormal basis for $K_r(A, b)$.
- Step 2: Find $\tilde{Q}_r \tilde{R}_r := \textcolor{brown}{A}Q_r$.
- Step 3: Solve $\tilde{R}_r c_r = \tilde{Q}_r^T b$ and set $x_r := Q_r c_r$.

Crucial: We can iteratively compute step 1 and step 2, i.e., use Q_{r-1} , \tilde{R}_{r-1} , \tilde{Q}_{r-1} to obtain Q_r , \tilde{R}_r , \tilde{Q}_r !

GMRES – Step 1 “Find an orthonormal basis for $K_r(A, b)$ ”

Given $Q_{r-1} = (q_1, \dots, q_{r-1}) \in \mathbb{R}^{n \times (r-1)}$ with $\text{Im}(Q_{r-1}) = K_{r-1}(A, b)$ from the previous iteration step, let us compute

$$q_r := \text{Arnoldi_step}(q_1, \dots, q_{r-1}; Aq_{r-1}).$$

(“orthogonalizing Aq_{r-1} against all q_1, \dots, q_{r-1} by subtracting projections and normalization”)

We recall the r -th Arnoldi iteration step in an algorithmic fashion:

Given $q_1(:= \frac{b}{\|b\|}), \dots, q_{r-1}$, then q_r is computed by:

```

 $q_r := \text{Arnoldi\_step}(q_1, \dots, q_{r-1}; v = Aq_{r-1}):$ 
    for  $\ell = 1, \dots, r-1$  do
         $h_{\ell, r-1} = q_{\ell}^T v$ 
         $v = v - h_{\ell, r-1} q_{\ell}$    (subtracting projections)
    end
     $h_{r, r-1} = \|v\|$ 
    if  $h_{r, r-1} \neq 0$  then
         $q_r = \frac{v}{h_{r, r-1}}$            (normalization)
        return  $q_r$ 
    end
return  $v$ 
```

In matrix notation this can be summed up as follows:

$$A \cdot \underbrace{\begin{pmatrix} | & & | \\ q_1 & \cdots & q_{r-1} \\ | & & | \end{pmatrix}}_{=:Q_{r-1} \in \mathbb{R}^{n \times (r-1)}} = \underbrace{\begin{pmatrix} | & & | \\ Aq_1 & \cdots & Aq_{r-1} \\ | & & | \end{pmatrix}}_{\text{Arnoldi: } Aq_j = \sum_{\ell=1}^{j+1} h_{\ell,j} q_{\ell}} = \underbrace{\begin{pmatrix} | & & | & | \\ q_1 & \cdots & q_{r-1} & q_r \\ | & & | & | \end{pmatrix}}_{=:Q_r \in \mathbb{R}^{n \times r}} \underbrace{\begin{pmatrix} h_{1,1} & h_{1,2} & \cdots & & \\ h_{2,1} & h_{2,2} & & & \\ 0 & h_{3,2} & & & \\ \vdots & 0 & \ddots & h_{r-1,r-2} & h_{r-1,r-1} \\ 0 & 0 & 0 & h_{r,r-2} & h_{r,r-1} \end{pmatrix}}_{=:H_{r,r-1} \in \mathbb{R}^{r \times (r-1)}}$$

$$\overset{Q_{r-1}^T \cdot |}{\Leftrightarrow} Q_{r-1}^T A Q_{r-1} = Q_{r-1}^T Q_r H_{r,r-1} = \begin{pmatrix} & & | & 0 \\ & & I_{(r-1) \times (r-1)} & \vdots \\ & & | & 0 \end{pmatrix} \begin{pmatrix} & H_{r-1} \\ & \cdots \\ \text{row } r \text{ of } H_{r,r-1} \end{pmatrix} = H_{r-1}$$

- We observe that $H_{r-1} \in \mathbb{R}^{(r-1) \times (r-1)}$ has only one subdiagonal. Such matrices are called (upper) **Hessenberg matrices**.
- In particular, for $r = n + 1$, we find

$$Q_n^T A Q_n = H_n \in \mathbb{R}^{n \times n}.$$

With other words, with the help of the Arnoldi iteration we can find in finitely many steps (at most n steps) an upper Hessenberg H_n , which is orthogonally similar to A and thus has the same eigenvalues. That is why one can tailor the QR-algorithm (which was an algorithm to compute eigenvalues) to matrices of Hessenberg structure. The Arnoldi iteration is therefore also considered an eigenvalue algorithm. Furthermore, if A is symmetric, so is H_n , which then becomes a tridiagonal matrix.

GMRES – Step 2 “Compute QR-decomposition $\tilde{Q}_r \tilde{R}_r := A Q_r$ ”

Again, we want to rely on the computations from the previous steps, i.e., $\tilde{Q}_{r-1} = [\tilde{q}_1, \dots, \tilde{q}_{r-1}] \in \mathbb{R}^{n \times (r-1)}$ and $\tilde{R}_{r-1} = [\tilde{r}_1, \dots, \tilde{r}_{r-1}] \in \mathbb{R}^{(r-1) \times (r-1)}$ with $\tilde{Q}_{r-1} \tilde{R}_{r-1} = A Q_{r-1}$. Therefore, let us first observe that

$$\tilde{Q}_r \tilde{R}_r \stackrel{!}{=} A Q_r = A \cdot [Q_{r-1} | q_r] = [A Q_{r-1} | A q_r] = [\tilde{Q}_{r-1} \tilde{R}_{r-1} | A q_r] \in \mathbb{R}^{n \times r}.$$

Let us use one Arnoldi step to orthogonalize $A q_r$ against $\tilde{q}_1, \dots, \tilde{q}_{r-1}$ to obtain

$$\tilde{q}_r, \tilde{r}_r := \text{Arnoldi_step}(\tilde{q}_1, \dots, \tilde{q}_{r-1}; A q_r),$$

where the vector \tilde{q}_r and the coefficients of $\tilde{r}_r = (\tilde{r}_{1,r}, \dots, \tilde{r}_{r,r})^\top \in \mathbb{R}^r$ are computed via

$$\hat{q}_r := A q_r - \sum_{j=1}^{r-1} \tilde{r}_{j,r} \cdot \tilde{q}_j, \quad \tilde{r}_{j,r} := \tilde{q}_j^\top (A q_r), \quad \tilde{q}_r := \frac{\hat{q}_r}{\|\hat{q}_r\|_2}, \quad \tilde{r}_{rr} := \|\hat{q}_r\|_2,$$

from which we can conclude

$$A q_r = \tilde{r}_{rr} \tilde{q}_r + \sum_{j=1}^{r-1} \tilde{r}_{j,r} \tilde{q}_j = \sum_{j=1}^r \tilde{r}_{j,r} \tilde{q}_j. \quad (*)$$

Then let us define potential candidates for the sought-after QR-decomposition as follows:

$$\tilde{Q}_r := [\tilde{Q}_{r-1} | \tilde{q}_r], \quad \tilde{R}_r := \begin{pmatrix} \tilde{R}_{r-1} & | \\ \cdots & \tilde{r}_r \\ 0 \cdots 0 & | \end{pmatrix} \in \mathbb{R}^{r \times r}.$$

By $(*)$ we can write $A q_r = \tilde{Q}_r \tilde{r}_r$ and indeed find, as desired,

$$A Q_r = (A Q_{r-1} | A q_r) = (\tilde{Q}_{r-1} \tilde{R}_{r-1} | \tilde{Q}_r \tilde{r}_r) = \tilde{Q}_r \tilde{R}_r.$$

GMRES – Step 3 “Solve a triangular system”

The last step is easily performed by invoking a routine to solve the upper triangular system

$$\tilde{R}_r c_r = \tilde{Q}_r^T b$$

via backward substitution. Then we find our r -th iterate by setting

$$x_r := Q_r c_r.$$

5.2.4 Summary and final Remarks: GMRES with Arnoldi

- i) We only need one matrix-vector product $v \mapsto Av$ in each step! This product can be delivered to the solver GMRES as some sort of black box function.
- ii) **An initial guess** $x_0 \neq 0$:

Consider

$$x_r := x_0 + p_r, \quad \text{for some } x_0 \neq 0,$$

then

$$Ax_r = b \Leftrightarrow A(x_0 + p_r) = b \Leftrightarrow Ap_r = b - Ax_0 = \hat{b}.$$

Then we could solve the auxiliary system to obtain $p := \text{GMRES}(A, \hat{b})$ and set $x := x_0 + p$. The above algorithm can therefore easily be extended to allow for an initial guess x_0 other than the zero vector. Also note that the Krylov subspaces are then generated based on the initial residual $\hat{b} = b - Ax_0$.

- iii) **Preconditioning:**

Let us consider $N \in \text{GL}_n(\mathbb{R})$, $N \approx A^{-1}$, where $v \mapsto Nv$ is also easy to compute. Then

$$Ax = b \Leftrightarrow \underbrace{NA}_{=: \tilde{A}} x = \underbrace{Nb}_{=: \tilde{b}} \Leftrightarrow \tilde{A}x = \tilde{b}.$$

Then we could solve the equivalent system to obtain $x := \text{GMRES}(\tilde{A}, \tilde{b})$.

What is actually a good precondition? Quite a bit of research has been put into this question over the last decades. What one can say: Krylov subspace methods converge quickly if the eigenvalues appear in clusters away from zero.

iv) **Restarted GMRES:**

- We need to store $Q_r := (q_1, \dots, q_r)$, $\tilde{Q}_r := (\tilde{q}_1, \dots, \tilde{q}_r)$ and $\tilde{R}_r := (\tilde{r}_1, \dots, \tilde{r}_r)$. Thus, if the above algorithm runs many iterations, then Q_r, \tilde{Q}_r may become large (usually dense) matrices ($n \gg 1$), then the advantage of the sparsity of A is lost.
- Idea: Perform only a fixed number of iterations, say $m = 20 - 40$ and then restart GMRES with initial guess x_m . The resulting algorithm is sometimes coined GMRES(m). You will later learn about a similar idea in the context of the L-BFGS method.
- Remark: If A is symmetric and positive definite, then one can show that we do not need the whole history q_1, \dots, q_r . This is the power of the CG-method which you will investigate next semester.

v) **Another perspective and variant:** Let us consider

$$\begin{aligned} \min_{x_r \in K_r(A, b)} \|Ax_r - b\|_2^2 &= \min_{c_r \in \mathbb{R}^r} \|AQ_r c_r - b\|_2^2 = \min_{c_r \in \mathbb{R}^r} \|Q_{r+1} H_{r+1,r} c_r - b\|_2^2 \\ &\stackrel{(\#)}{=} \min_{c_r \in \mathbb{R}^r} \underbrace{\|H_{r+1,r} c_r - \begin{pmatrix} \|b\| \\ 0 \\ \vdots \\ 0 \end{pmatrix}\|_2^2}_{\text{we can evaluate this residual without computing } x_r!} \quad (*) \end{aligned}$$

$$(\#): q_1 := \frac{b}{\|b\|} \Rightarrow b = q_1 \|b\| \Rightarrow Q_{r+1}^T b = \begin{pmatrix} \|b\| \\ 0 \\ \vdots \\ 0 \end{pmatrix} \Rightarrow b = Q_{r+1} \begin{pmatrix} \|b\| \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

Let $\widehat{Q}_{r+1}\widehat{R}_r := H_{r+1,r}$ be a QR-decomposition, then the normal equation associated to (*) could be solved by:

$$\widehat{R}_r c_r = \widehat{Q}_{r+1}^T \begin{pmatrix} \|b\| \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

This results in a different variant of the GMRES and the following adaptions would apply:

- In step 2: We could derive such a QR-decomposition $\widehat{Q}_{r+1}\widehat{R}_r := H_{r+1,r}$ from our arrays by setting

$$\widehat{Q}_{r+1} := Q_{r+1}^T \widetilde{Q}_r, \quad \widehat{R}_r := \widetilde{R}_r$$

because then

$$\widetilde{Q}_r \widetilde{R}_r \stackrel{!}{=} A Q_r = Q_{r+1} H_{r+1,r} \Leftrightarrow Q_{r+1}^T \widetilde{Q}_r \widetilde{R}_r = H_{r+1,r} \Leftrightarrow \widehat{Q}_{r+1} \widehat{R}_r = H_{r+1,r} \quad (*).$$

- In step 3: Our normal equation could then be written as

$$\widetilde{R}_r c_r = \widetilde{Q}_r^T b \Leftrightarrow \widetilde{R}_r c_r = (Q_{r+1}^T \widetilde{Q}_r)^T \begin{pmatrix} \|b\| \\ 0 \\ \vdots \\ 0 \end{pmatrix} \Leftrightarrow \widehat{R}_r c_r = \widehat{Q}_{r+1} \begin{pmatrix} \|b\| \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

All in all we obtain the following algorithm:

INPUT: $A \in GL_n(\mathbb{R})$, $b \in \mathbb{R}^n$

OUTPUT: approximation $x_r \in K_r(A, b)$ to the exact solution $A^{-1}b$

GMRES($A, b, x_0 = 0, \text{tol} = 1e-6, \text{maxiter=None}, N = I$):

$b = b - Ax_0$ //account for initial guess

$A = NA, b = Nb$ //account for preconditioner

//Initialization:

$q_1 := \frac{b}{\|b\|_2}, Q_1 := [q_1]$

$v := Aq_1, \tilde{q}_1 := \frac{v}{\|v\|_2}, \tilde{Q}_1 := [\tilde{q}_1], \tilde{R}_1 = [\|v\|_2]$

for $r = 2, \dots, \min(n, \text{maxiter})$ **do**

//STEP 1: use Arnoldi to find column q_r by orthogonalizing v against q_1, \dots, q_{r-1}

$q_r, h_{r-1} := \text{Arnoldi_step}(Q_{r-1}; v)$ //we don't need h_{r-1}

$Q_r := [Q_{r-1}, q_r]$

$v := Aq_r$

//STEP 2: use Arnoldi to find columns \tilde{q}_r, \tilde{r}_r by orthogonalizing v against $\tilde{q}_1, \dots, \tilde{q}_{r-1}$

$\tilde{q}_r, \tilde{r}_r := \text{Arnoldi_step}(\tilde{Q}_{r-1}; v)$

$\tilde{Q}_r := [\tilde{Q}_{r-1}, \tilde{q}_r], \tilde{R}_r := [\tilde{R}_{r-1}, \tilde{r}_r]$

//STEP 3: solve auxiliary least squares problems to obtain coordinates

$c_r := \text{solve_triangular}(\tilde{R}_r, \tilde{Q}_r^\top b)$

$x_r := Q_r c_r$

//Attention: Evaluate the original residual here:

if $\|N^{-1}(Ax_r - b)\|_2 < \text{tol}$ **then**

| break

end

end

return $x_r + x_0$

Least Squares Problems

Recommended reading:

- Lecture 11 in [4]
- Section II.2 in [3]
- This handout by Homer F. Walker:
https://users.wpi.edu/~walker/MA3257/HANDOUTS/least-squares_handout.pdf

- [1] R. Rannacher.
Numerik 0 - Einführung in die Numerische Mathematik.
Heidelberg University Publishing, 2017.
- [2] G. Strang.
Introduction to Linear Algebra.
Wellesley-Cambridge Press, 2003.
- [3] G. Strang.
Linear Algebra and Learning from Data.
Wellesley-Cambridge Press, 2019.
- [4] L.N. Trefethen and D. Bau.
Numerical linear algebra.
SIAM, Soc. for Industrial and Applied Math., Philadelphia, 1997.

6 Least Squares Problems

6.1 Overview

OVERVIEW: Given $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$, find $x \in \mathbb{R}^n$
such that

$$\underbrace{Ax - b = 0}_{\text{Interpolation}}, \quad \underbrace{Ax - b \approx 0}_{\text{Regression}}$$

Solution set $\hat{S} := \{x \in \mathbb{R}^n : Ax = b\} = f_A^{-1}(\{b\})$
($\text{Im } A = \{Ax : x \in \mathbb{R}^n\}$)

b .

a_1^T
 ~~a_2^T~~
 a_n^T

$|S| \in \{0, 1, \infty\}$
 $|S| = 0$ $(b \notin \text{Im } A)$
 $|S| = 1$ (col. are ind.)
 $|S| = \infty$ (col. are dep.)

(EXISTENCE)

REFORMULATION
TO ENFORCE
EXISTENCE

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2$$

$$S := \{x \in \mathbb{R}^n : x = \arg \min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2\}$$

$|S| = 1$
(col. are ind.)

$|S| = \infty$
(col. are dep.)

REFORMULATION
TO ENFORCE
UNIQUENESS

- REGULARIZATION
- MINIMUM NORM LS-SOLUTIONS

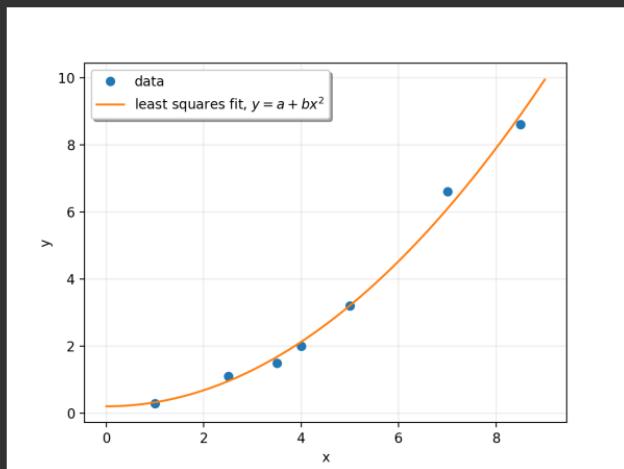
$= 1$ ($S = \hat{S}$)
UNIQUENESS
 ∞ ($S = \hat{S}$)
($b \in \text{Im } A$)
(columns are dep.)

Situation: We allow for $b \notin \text{Im}(A)$

⇒ The system $Ax = b$ is not solvable, i.e., there is **no** $x^* \in \mathbb{R}^n$ so that $Ax^* = b$

Example: Curve fitting

The situation above typically occurs when trying to explain a set of data by just a few parameters leading to over-determined systems: more equations than unknowns ($m \gg n$).



Corresponding system:

$$\begin{pmatrix} 1 & z_1^2 \\ \vdots & \vdots \\ 1 & z_n^2 \end{pmatrix} \begin{pmatrix} a \\ b \end{pmatrix} = \begin{pmatrix} y_1 \\ \vdots \\ y_n \end{pmatrix}$$

Approach: Minimize the error (/residual/defect) $\|Ax - b\|$

We obtain existence by reformulating the problem:

Definition 6.1 (Least Squares Solution) Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^n$. Then $\hat{x} \in \mathbb{R}^n$ is called a **least squares solution of $Ax = b$** , if \hat{x} is a minimizer of the problem

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2,$$

i.e., $\|A\hat{x} - b\|_2^2 \leq \|Ax - b\|_2^2$ for all $x \in \mathbb{R}^n$.

Remark

- We recall that $\|x\|_2 := \sqrt{\sum_{i=1}^n x_i^2}$ which explains the naming:

$$\|Ax - b\|_2^2 = \sum_{i=1}^m (\underbrace{\dots}_\text{"squares"})^2 \rightarrow \underbrace{\min}_{\text{"least squares"}}$$

- The norm is always nonnegative, i.e., $\|x\|_2 \geq 0$, so that the minimal possible value of the objective function is zero (which would imply $Ax = b$ due to the definiteness of the norm).
- Also, since squaring $x \mapsto x^2$ is a monotonically increasing function on nonnegative numbers we can minimize the squared residual without changing the set of minimizers, i.e.,

$$\hat{S} := \{x \in \mathbb{R}^n : x := \arg \min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2\} = \{x \in \mathbb{R}^n : x := \arg \min_{x \in \mathbb{R}^n} \|Ax - b\|_2\}.$$

As a result we get rid of the square root which is advantageous in terms of derivatives (see optimality conditions later). Note that the optimal value of the objective function may differ, but this is not important here.

6.2 The Normal Equation

The minimization problem is equivalent to a linear system:

Theorem 6.2 (Normal Equation) Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. Then $\hat{x} \in \mathbb{R}^n$ is a least squares solution of $Ax = b$ if and only if \hat{x} solves the **normal equation**

$$A^T A \hat{x} = A^T b.$$

Proof sketch:

(1) *Optimization perspective:*

Let us define the objective function

$$f: \mathbb{R}^n \rightarrow \mathbb{R}, \quad f(x) := \|Ax - b\|_2^2.$$

Then one can show that f is convex, i.e.,

$$f(\lambda x_1 + (1 - \lambda)x_2) \leq \lambda f(x_1) + (1 - \lambda)f(x_2) \quad \forall \lambda \in [0, 1].$$

In fact, this is an immediate consequence of the triangle inequality and the absolute homogeneity of the norm as well as the monotonicity of the square.

The convexity of the objective function then implies the existence of a minimizer as well as the necessary *and* sufficient first-order optimality condition:

$$\hat{x} \text{ minimizer} \iff 0 = f'(\hat{x}) = 2A^T(A\hat{x} - b) \quad (\text{normal equation}).$$

(2) Geometric Perspective:

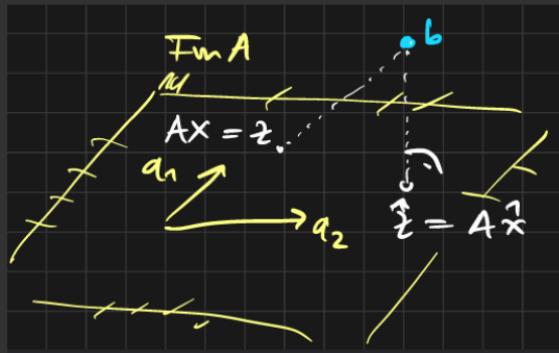
We recall that

$$\text{Im}(A) = \{Ax : x \in \mathbb{R}^n\} = \text{span}(a_1, \dots, a_n) = \{x_1 a_1 + \dots + x_n a_n : x \in \mathbb{R}^n\} \subset \mathbb{R}^m.$$

Therefore the least squares problem also reads as

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2 = \min_{z \in \text{Im}(A)} \|z - b\|_2^2.$$

Example: Let $A \in \mathbb{R}^{3 \times 2}$ and $b \in \mathbb{R}^3$.



- The point $\hat{z} \in \mathbb{R}^m$ is the point in the plane $\text{Im}(A)$, which is as close as possible to b in terms of the Euclidean norm $\|\cdot\|_2$.
→ The vector $(\hat{z} - b)$ is orthogonal to this plane!
- By definition of the image $\text{Im}(A)$, each z in this plane can be written as $z = Ax$ for some $x \in \mathbb{R}^n$.
- The parameter vector \hat{x} with $\hat{z} = A\hat{x}$ is the desired least squares solution.

One can show that the orthogonal projection yields shortest distance:

Lemma 6.3 (Orthogonal Projection) Let $V \subset \mathbb{R}^m$ be a linear subspace and $b \in \mathbb{R}^m$. Then

$$\hat{z} = \arg \min_{z \in V} \|z - b\|_2^2 \quad \Leftrightarrow \quad \hat{z} - b \in V^\perp := \{w \in \mathbb{R}^n : w^\top z = 0 \quad \forall z \in V\}, \quad \hat{z} \in V.$$

Proof. The following equation is crucial for the proof (compare Pythagorean identity): Let $\hat{z} \in V$ be fixed, then for all $z \in V$ we have

$$\begin{aligned} \|z - b\|_2^2 &= \|b - \hat{z} + \hat{z} - z\|_2^2 \\ &= \|b - \hat{z}\|_2^2 + \|\hat{z} - z\|_2^2 + 2(b - \hat{z})^\top(z - \hat{z}) \end{aligned} \tag{13}$$

Exemplary, we only proof direction " \Leftarrow " here.

Now let $\hat{z} - b \in V^\perp$, so that $\forall z \in V$,

$$(\hat{z} - b)^\top(z - \hat{z}) = 0.$$

Inserting this into equation (??) and exploiting the positivity of the norm we thus obtain

$$\begin{aligned} \|z - b\|_2^2 &= \|b - \hat{z}\|_2^2 + \|\hat{z} - z\|_2^2 + 2(b - \hat{z})^\top(z - \hat{z}) \\ &= \|b - \hat{z}\|_2^2 + \|\hat{z} - z\|_2^2 \\ &\geq \|b - \hat{z}\|_2^2, \end{aligned}$$

for all $z \in V$.

The reverse direction also relies on (??). See, e.g., the third proof in this Wikipedia section. □

Now let us apply this lemma to our setting $V = \text{Im}(A)$ and exploit the orthogonality of the fundamental subspaces ($\text{Im}(A)^\perp = \ker(A^\top)$). We obtain

$$\begin{aligned}\hat{z} = \arg \min_{z \in \text{Im}(A)} \|z - b\|_2^2 &\iff \hat{z} - b \in \text{Im}(A)^\perp = \ker(A^\top), \quad \hat{z} \in \text{Im}(A) \quad (\text{Lemma ??}) \\ &\iff A^\top(\hat{z} - b) = 0, \quad \hat{z} \in \text{Im}(A) \quad (\text{definition of } \ker(A^\top)) \\ &\iff A^\top(A\hat{x} - b) = 0 \quad \text{for some } \hat{x} \in \mathbb{R}^n \quad (\text{definition of } \hat{z} \in \text{Im}(A))\end{aligned}$$

- The normal equation then reads as:

The least squares solution \hat{x} is so that
the residual vector $A\hat{x} - b$ is orthogonal to all columns of A .

- We also find an equivalent characterization for the solution set, namely,

$$\hat{S} = \{x \in \mathbb{R}^n : A^T A x = A^T b\}.$$

Analysis of the Normal Equation

(1) Properties of the system matrix $A^T A$ (*Gramian matrix*)

- $A^T A$ is of size $n \times n$ (for typically $n \ll m$)
- $A^T A$ is symmetric and positive semi-definite (\Rightarrow nonnegative eigenvalues)
- $\ker(A) = \ker(A^T A)$, which implies:
 A independent columns $\iff \ker(A) = \{0\} \iff \ker(A^T A) = \{0\} \iff A^T A$ is invertible.

With other words, the least squares solution is unique if and only if A has independent columns (also compare to the geometric interpretation above).

(2) For any A, b there exists a least squares solution (existence enforced ✓)

Due to $\ker(A) = \ker(A^T A)$ and $\text{Im}(A) = \ker(A^T)^{\perp}$, we have

$$\begin{aligned}\text{existence: } \exists x \in \mathbb{R}^n : A^T A x = A^T b &\iff A^T b \in \text{Im}(A^T A) = \ker(A^T A)^{\perp} = \ker(A)^{\perp} \\ &\iff 0 = (A^T b)^T v = b^T (Av) \quad \forall v \in \ker(A)\end{aligned}$$

The latter statement on the right-hand side is true for any matrix A and any vector b .

(3) Consistent reformulation:

If $b \in \text{Im}(A)$, i.e., if the original system $Ax = b$ is solvable, then

$$\{x \in \mathbb{R}^n : Ax = b\} =: S = \widehat{S} := \{x \in \mathbb{R}^n : A^T A x = A^T b\}.$$

Proof:

- " $S \subset \widehat{S}$ ":

Let $x \in S = \{x \in \mathbb{R}^n : Ax = b\}$ (such an element x exists because we assume $b \in \text{Im}(A)$), then

$$Ax - b = 0 \stackrel{A^T \cdot |}{\Rightarrow} A^T(Ax - b) = 0 \Rightarrow x \in \widehat{S} = \{x \in \mathbb{R}^n : A^T A x = A^T b\}.$$

- " $\widehat{S} \subset S$ ":

Let $\widehat{x} \in \widehat{S}$, i.e., $\widehat{x} := \underset{x \in \mathbb{R}^n}{\operatorname{argmin}} \|Ax - b\|_2^2$, then because $b \in \text{Im}(A)$,

$$\|A\widehat{x} - b\|_2^2 = 0.$$

Thus

$$A\widehat{x} - b = 0 \Rightarrow \widehat{x} \in S.$$

6.3 Solving the Normal Equation

Assumptions:

- A has independent columns (existence and uniqueness ✓)
- n is of moderate size (direct methods applicable ✓)

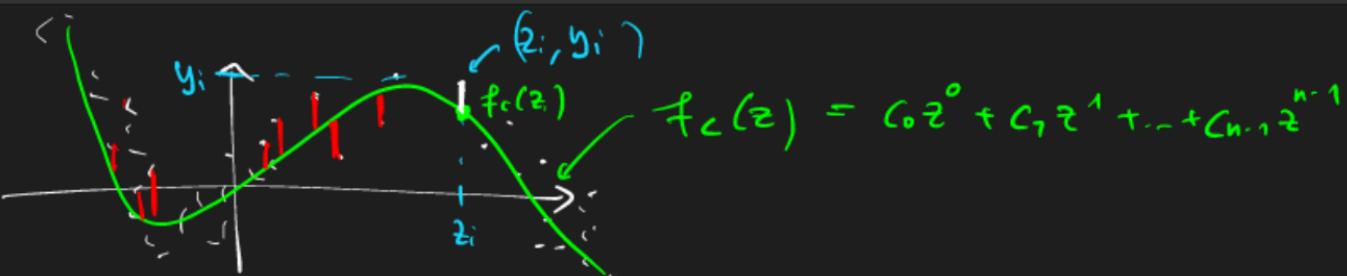
Thus there is a unique least squares solution given by (also revisit the section on projections)

$$\hat{x} = (A^T A)^{-1} A^T b.$$

Example: Polynomial regression

- Here we typically have many measurements $(z_1, y_1), \dots, (z_m, y_m) \in \mathbb{R}^2$ (i.e., m large).
- Polynomial model is given by $f_c(z) := \sum_{j=0}^{n-1} c_j z^j$ (for n rather small because we want to smoothen the data).
- The corresponding design matrix is then given by $A = (z_i^{j-1})_{ij}$ (revisit section on curve fitting).
- One can show:

If all the z_i are distinct, then the columns of A are independent (see Vandermonde matrix)!



Approaches:

(1) Using Cholesky decomposition $A^\top A = LL^\top$

→ Problem: $A^\top A$ often *ill-conditioned* and numerical elimination may fail due to rounding errors!

Can we work without $A^\top A$? Yes!

(2) Using reduced QR Decomposition $A = \widehat{Q}\widehat{R}$

Let us recall that

$$\forall A \in \mathbb{R}^{m \times n} \exists \widehat{Q} \in \mathbb{R}^{m \times n} \text{ orthonormal columns}, \widehat{R} \in \mathbb{R}^{n \times n} \text{ triangular} : A = \widehat{Q}\widehat{R}.$$

Now we insert $A = \widehat{Q}\widehat{R}$ into the normal equation to obtain

$$A^\top Ax = A^\top b \stackrel{A=\widehat{Q}\widehat{R}}{\Leftrightarrow} (\widehat{Q}\widehat{R})^\top(\widehat{Q}\widehat{R})x = (\widehat{Q}\widehat{R})^\top b \Leftrightarrow \widehat{R}^\top\widehat{Q}^\top\widehat{Q}\widehat{R}x = \widehat{R}^\top\widehat{Q}^\top b \Leftrightarrow \widehat{R}^\top\widehat{R}x = \widehat{R}^\top\widehat{Q}^\top b.$$

If A has independent columns, we know that \widehat{R} is invertible and so is \widehat{R}^\top . Thus we end up with the system

$$\widehat{R}x = \widehat{Q}^\top b$$

which can be solved via *backward substitution*.

Remarks:

- Recall: Using the reduced QR decomposition to solve $Ax = b$ results in the same system. Now we see that for the case $b \notin \text{Im}(A)$, we solve the normal equation.
- If the columns of A are independent, then \widehat{R} is invertible and without loss of generality one can require $r_{ii} > 0$, otherwise one multiplies the i -th column in \widehat{Q} and row in \widehat{R} by “ -1 ”. Thus, the factorization $\widehat{R}^\top\widehat{R}$ can be considered a Cholesky decomposition of $A^\top A$. However, the difference here is that we obtain it by the QR decomposition of A and not by applying the Cholesky algorithm to $A^\top A$. The former is roughly twice as expensive. One can show that this additional effort pays off in terms of improved stability against rounding errors.

(3) Using the Pseudoinverse A^+ (see below)

This is typically not done in practice since the computation of the singular value decomposition (which has to be iterative in higher dimensions since we need to solve eigenvalue problems) is more expensive than a direct method. However it offers interesting theoretical insights as we will see below.

(4) Randomized algorithms:

If $A^T A$ is large (n large), then in particular $A^T A$ cannot (and should not) be computed.

In such cases one can use *randomized* algorithms which only work with subsamples of the columns of A (not addressed in this course; see for example [3, II.4])

6.4 Regularization and Minimum Norm Least Squares Solution (enforce uniqueness)

6.4.1 Motivation and Overview

Situation: Columns of A are possibly linearly dependent ($\ker(A) \supsetneq \{0\}$)

$\Rightarrow A^T A$ not invertible

\Rightarrow there are infinitely many solutions of $A^T A x = A^T x$ (or if $b \in \text{Im}(A)$, of $Ax = b$)

- Geometric perspective:

Draw a picture with dependent columns of A and consider an example $b \in \text{Im}(A)$ and an example $b \notin \text{Im}(A)$.

- Algebraic perspective:

Let \hat{x} be a solution of the normal equation, then for all $x_0 \in \ker(A)$ we have that $\hat{x} + x_0$ is also a solution. In fact, we find

$$A^\top A(\hat{x} + x_0) = A^\top(A\hat{x} + Ax_0) = A^\top A\hat{x}.$$

\rightarrow We say the minimization problem is *ill-posed* (\neq well-posed = existence+uniqueness)

Question: Which solution to pick?

We briefly discuss two approaches: **Tikhonov Regularization** and **Minimum norm solution**

6.4.2 Tikhonov Regularization

Tikhonov Regularization of the least squares problem (*ridge regression*):

$$\min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2 + \frac{\delta}{2} \|x\|_2^2, \quad \text{for } \delta > 0 \text{ small.} \quad (14)$$

Remarks

- We enforce uniqueness by reformulating the problem. In fact, the idea here is to add a strictly convex regularization term $\frac{\delta}{2} \|x\|_2^2$ to the original objective function (*convexification*).
- The parameter $\delta > 0$ is sometimes called *regularization parameter*. The smaller it is, the closer do we get to the original problem, the more is the minimization of the residual emphasized.
- One can generalize the regularization term to a rather generic strictly convex function. Thereby one can control properties of the solution. For example, choosing the $\|\cdot\|_1$ - instead of the $\|\cdot\|_2$ -norm enforces sparsity on the solution, which is a desirable feature in many applications.

Characterization of the “regularized” solution

$$x_\delta := \arg \min_{x \in \mathbb{R}^n} \|Ax - b\|_2^2 + \frac{\delta}{2} \|x\|_2^2$$

Theorem 6.4 (“Regularized” Normal Equation) Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. Then $x_\delta \in \mathbb{R}^n$ solves the regularized problem (??) if and only if x_δ solves the “regularized” normal equation

$$(A^T A + \delta I)x = A^T b. \quad (15)$$

Proof:

Defining the (strictly convex) function $f(x) := \|Ax - b\|_2^2 + \frac{\delta}{2} \|x\|_2^2$, one can show for the sufficient and necessary first-order optimality conditions:

Analysis of the “regularized” normal equation

- The matrix $A^T A + \delta I$ is symmetric and positive definite *for all* $\delta > 0$ and thus **invertible**. More precisely:
 - Symmetry: (*Recall: A matrix B is called symmetric, if $B^T = B$ holds.*)
$$(A^T A + \delta I)^T = (A^T A)^T + \delta I^T = A^T A + \delta I$$
 - Positivity (*Recall: A matrix B is called positive definite, if $x^T B x > 0$ holds $\forall x \in \mathbb{R}^n$.*)
$$x^T (A^T A + \delta I) x = \underbrace{x^T (A^T A) x}_{\geq 0} + \underbrace{\delta}_{> 0} \underbrace{x^T x}_{> 0} > 0 \text{ for all } x \in \mathbb{R}^n \setminus \{0\}$$

Therefore, the equation (??) has the unique solution

$$x_\delta = (A^T A + \delta I)^{-1} A^T.$$

- The smaller δ , the more is the error minimization emphasized, the more do we approach the normal equation.
- We note that the vector x_δ (for $\delta > 0$) does neither solve $Ax = b$ nor $A^T A x = A^T b$!

6.4.3 Minimum Norm Solution and the Moore–Penrose Pseudoinverse

Idea: Among the infinitely many solutions we pick the one with *smallest* norm, i.e.,

$$\min_{x \in \hat{S}} \|x\|_2^2 \quad (\hat{S} := \{x \in \mathbb{R}^n : A^T Ax = A^T b\}). \quad (16)$$

→ We enforce uniqueness by determining a specific selection criterion.

Characterization of the minimum-norm solution

$$x^+ := \arg \min_{x \in \hat{S}} \|x\|_2^2$$

Theorem 6.5 (Minimum-Norm Least Squares) Let $A \in \mathbb{R}^{m \times n}$ and $b \in \mathbb{R}^m$. Then

$$x^+ = \lim_{\delta \rightarrow 0} x_\delta$$

solves the minimum-norm least squares problem (??). Here, $x_\delta = (A^T A + \delta I)^{-1} A^T b$ is the solution of the regularized least squares problem (??).

Proof: Uses the singular value decomposition.

Remarks

- By construction x^+ has two properties:

1) It is a least squares solution, i.e.,

$$A^T A x^+ = A^T b \quad (\text{or if } b \in \text{Im}(A), \text{ also } A x^+ = b).$$

2) It is the one with smallest norm, i.e.,

$$\|x^+\|_2 \leq \|\hat{x}\|_2 \quad \forall \hat{x} \in \hat{S}.$$

- By applying Theorem ?? we find

$$x^+ = \lim_{\delta \rightarrow 0} x_\delta = \lim_{\delta \rightarrow 0} (A^T A + \delta I)^{-1} A^T b = \left(\lim_{\delta \rightarrow 0} (A^T A + \delta I)^{-1} A^T \right) b.$$

- One can show that the limiting matrix

$$A^+ := \lim_{\delta \rightarrow 0} (A^T A + \delta I)^{-1} A^T$$

is precisely the so-called *Moore–Penrose Pseudoinverse* of A (proof below). With the help of the SVD $U\Sigma V^\top = A$, it can be computed by

$$A^+ = V \Sigma^+ U^\top,$$

where the pseudoinverse of a diagonal matrix $\Sigma = \text{diag}(\sigma_1, \dots, \sigma_r, 0, \dots, 0)$ is given by

$$\Sigma^+ = \text{diag}\left(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_r}, 0, \dots, 0\right).$$

The Moore–Penrose Pseudoinverse

Let us explain why the term *pseudoinverse* is used here.

Let $A \in \mathbb{R}^{m \times n}$ with $m \neq n$, then A and the corresponding function $f_A: \mathbb{R}^n \rightarrow \mathbb{R}^m$ can't be invertible. In fact, there can't be a one-to-one relation between the spaces \mathbb{R}^n and \mathbb{R}^m in this case.

- The two spaces have different dimensions. For instance, a single nonzero vector can explain a line (\mathbb{R}), but two independent vectors are needed to explain a plane (\mathbb{R}^2).
- One could say that \mathbb{R}^n and \mathbb{R}^m are “differently large” if $m \neq n$.

However: We still aim at solving systems $Ax = b$ for $A \in \mathbb{R}^{m \times n}$ with possibly $m \neq n$.

Recall: If A is invertible (then in particular $m = n$), then $x = A^{-1}b$ is the unique solution. The inverse is a function which maps the right-hand side to the unique solution.

- As seen above, the concept of an inverse matrix fails if $m \neq n$.

The minimum-norm least squares solution is a generally applicable concept which maps a right-hand side to “some sort of *unique* solution”:

$$x^+ := x^+(b) := \arg \min_{\substack{s.t. \\ A^T A x = A^T b}} \|x\|_2^2 = \left(\lim_{\delta \rightarrow 0} (A^T A + \delta I)^{-1} A^T \right) b \quad (x^+ \text{ uniquely exists!})$$

We finally show

i) The limiting matrix is the Moore–Penrose Pseudoinverse:

$$A^+ := \lim_{\delta \rightarrow 0} (A^T A + \delta I)^{-1} A^T = V \Sigma^+ U^\top$$

ii) Applying the Moore–Penrose Pseudoinverse to b gives the minimum-norm least squares solution:

$$x^+ = V \Sigma^+ U^\top b.$$

To i)

Let us consider the SVD $A = U \Sigma V^\top$, then

$$A^T A + \delta I = V (\Sigma^\top \Sigma + \delta^2 I) V^\top,$$

where

$$\Sigma^\top \Sigma + \delta^2 I = \text{diag}(\sigma_1^2 + \delta^2, \dots, \sigma_r^2 + \delta^2, \delta^2, \dots, \delta^2)$$

with inverse

$$(\Sigma^\top \Sigma + \delta^2 I)^{-1} = \text{diag}(1/(\sigma_1^2 + \delta^2), \dots, 1/(\sigma_r^2 + \delta^2), 1/\delta^2, \dots, 1/\delta^2)$$

Thus

$$(A^T A + \delta I)^{-1} A^T = V [(\Sigma^\top \Sigma + \delta^2 I)^{-1} \Sigma^\top] V^\top$$

where

$$(\Sigma^\top \Sigma + \delta^2 I)^{-1} \Sigma^\top = \text{diag}\left(\frac{\sigma_1}{\sigma_1^2 + \delta^2}, \dots, \frac{\sigma_r}{\sigma_r^2 + \delta^2}, 0, \dots, 0\right) \rightarrow \text{diag}\left(\frac{1}{\sigma_1}, \dots, \frac{1}{\sigma_r}, 0, \dots, 0\right) = \Sigma^+$$

for $\delta \rightarrow 0$.

To ii) 1. Let us start with the simple case: $A \in \mathbb{R}^{m \times n}$ diagonal

$$A = \begin{pmatrix} a_{11} & & & 0 \\ & \ddots & & \\ & & a_{rr} & \\ & & 0 & \ddots \\ 0 & & & 0 \end{pmatrix} \in \mathbb{R}^{m \times n}, \quad a_{ii} \neq 0, \quad A^T A = \begin{pmatrix} a_{11}^2 & & & 0 \\ & \ddots & & \\ & & a_{rr}^2 & \\ & & 0 & \ddots \\ 0 & & & 0 \end{pmatrix} \in \mathbb{R}^{n \times n}$$

Normal equation:

$$A^T A x = A^T b = \begin{pmatrix} a_{11} b_1 \\ \vdots \\ a_{rr} b_r \\ 0 \\ \vdots \\ 0 \end{pmatrix} \Leftrightarrow \begin{array}{l} a_{11}^2 x_1 = a_{11} b_1 \\ \vdots \\ a_{rr}^2 x_r = a_{rr} b_r \\ 0 \cdot x_i = 0 \\ \quad (i > r) \end{array} \Leftrightarrow \begin{array}{l} x_1 = \frac{b_1}{a_{11}} \\ \vdots \\ x_r = \frac{b_r}{a_{rr}} \\ x_{r+1} = 0 \\ \vdots \\ x_n = 0 \end{array}$$

$$\Rightarrow x^+ = \begin{pmatrix} \frac{1}{a_{11}} b_1 \\ \vdots \\ \frac{1}{a_{rr}} b_r \\ 0 \\ \vdots \end{pmatrix} 0 = A^+ b, \quad A^+ = \begin{pmatrix} \frac{1}{a_{11}} & & & 0 \\ & \ddots & & \\ & & \frac{1}{a_{rr}} & \\ & & 0 & \ddots \\ 0 & & & 0 \end{pmatrix} \in \mathbb{R}^{n \times m}$$

Note: The x_i for $i > r$ can be chosen arbitrarily, but setting them to zero gives the smallest vector.

2. Now we use these ideas for the general case: $A \in \mathbb{R}^{m \times n}$

By using the SVD $A = U\Sigma V^\top$ we find

$$A^T A = (U\Sigma V^\top)^T U\Sigma V^\top = V\Sigma^T \Sigma V^\top,$$

so that the normal equation reads as

$$\begin{aligned} (*) \quad A^T A x &= A^T b \Leftrightarrow V\Sigma^T \Sigma (V^\top x) = V\Sigma^T (U^\top b) \\ &\stackrel{V^\top \cdot |}{\Leftrightarrow} \underbrace{\Sigma^T \Sigma (V^\top x)}_{(\text{normal equation for } (\Sigma, U^\top b))} = \Sigma^T (U^\top b) \quad (\sharp) \end{aligned}$$

Consequently, x solves $(*)$ if and only if $y := V^\top x$ solves (\sharp) . Since V is orthogonal, both solutions have the same norm, more precisely,

$$\|x\|_2^2 = x^\top x = x^\top (VV^\top)x = \|V^\top x\|_2^2 = \|y\|_2^2.$$

From 1. above on diagonal matrices we know that $y^+ = \Sigma^+ U^\top b$ is the smallest solution of (\sharp) . Thus, $x^+ := Vy^+ = V\Sigma^+ U^\top b = A^+ b$ is the smallest solution of $(*)$, i.e., the minimum norm least squares solution.

All in all: Since orthogonal matrices (here U and V) are not only invertible but also isometric and the SVD $A = U\Sigma V^\top$ always exists, we could rely on the result for diagonal matrices (here Σ).

6.5 Small Tour: Inverse Problems in Imaging

→ presented in an ipython notebook.

Vector Spaces

7 Vector Spaces

7.1 Introduction

Preliminary remarks:

- So far, we worked with “vectors” in $\mathbb{R}^n, \mathbb{F}^n, \dots$. We introduced the notions of summation, multiplication, linear combination, span, basis,...
- We also summed and scaled matrices, but did not talk about a span of matrices, basis, etc...
- In the exercise class we considered infinite discrete signals. We could add and scale sequences in $\mathbb{R}^{\mathbb{N}}, \mathbb{R}^{\mathbb{Z}}, \dots$ as well and talk about linear combinations, basis, etc...
- Similarly, considering functions $f: \mathbb{R} \rightarrow \mathbb{R}$ and sets of functions (function spaces are studied in functional analysis). We could define summation and scaling. Example: Polynomials, frequencies,...

We now establish a more abstract point of view and revisit notions such as vectors, linear combinations, basis, etc. once again. You will see that we have already learned all the basic ideas.

Definition 7.1 (Group) Let G be a set and $* : G \times G \rightarrow G$ a function, so that

G1 Associativity: $\forall g_1, g_2, g_3 \in G : g_1 * (g_2 * g_3) = (g_1 * g_2) * g_3$

G2 Neutral element: $\exists e \in G \forall g \in G : g * e = g$

G3 Inverse element: $\forall g \in G \exists g^{-1} \in G : g * g^{-1} = e$

Then $(G, *)$ is called **group**.

If in addition

G4 Commutativity: $\forall g_1, g_2 \in G : g_1 * g_2 = g_2 * g_1$,

then it is called a **commutative/abelian group**.

Group theory plays a crucial role in cryptography (RSA,...)

Example 7.2

- $G = \{g\}$
- $(\mathbb{Z}, +)$
- $(\text{GL}(n, \mathbb{R}), \cdot)$; it is not commutative, take e.g.,

$$\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix}$$

In words: If both coordinates are scaled differently, then it makes a difference if we swap them before or after the scaling.

Not a group:

- $(\mathbb{N}, +)$, inverse element of 1?

We now add more structure by abstracting the familiar properties of real numbers with summation (subtraction) and multiplication (division).

Definition 7.3 (Field) Let F be a set and $+ : F \times F \rightarrow F$ and $\cdot : F \times F \rightarrow F$ two functions such that

F1 $(F, +)$ is a commutative group (with neutral element 0)

F2 $(F \setminus \{0\}, \cdot)$ is a commutative group (with neutral element 1)

F3 Distributivity (compatibility of $+$ and \cdot)

$$a \cdot (b + c) = a \cdot b + a \cdot c$$

$$(a + b) \cdot c = a \cdot c + b \cdot c$$

Example 7.4

- $(\mathbb{R}, +, \cdot)$
- $(\mathbb{Q}, +, \cdot)$
- $(\mathbb{C}, +, \cdot)$

Not a field:

- $(\mathbb{Z}, +, \cdot)$, because $(\mathbb{Z} \setminus \{0\}, \cdot)$ is not a group (no multiplicative inverse of, e.g., 2, 3, 4...)
It is just a "ring" (with respect to multiplication it is a semigroup (no inverses) and not a group)

We now abstract the notion of vectors in \mathbb{R}^n and their properties.

Definition 7.5 (Vector space) Let \mathbb{F} be a field. A set V together with a function $+$ (sum) and a function \cdot (scalar multiplication) with

$$\begin{aligned} + : V \times V &\rightarrow V & \cdot : \mathbb{F} \times V &\rightarrow V \\ (v, w) &\mapsto v + w & (\lambda, v) &\mapsto \lambda \cdot v \end{aligned}$$

is called **vector space (or linear space)** over \mathbb{F} , if the following axioms **VR1** and **VR2** hold:

VR1 $(V, +)$ is a commutative group with neutral element 0.

VR2 The scalar multiplication is compatible with $(V, +)$ in the following way:
for $\lambda, \mu \in \mathbb{F}, v, w \in V$ it holds that

- i) $(\lambda + \mu) \cdot v = \lambda \cdot v + \mu \cdot v$
- ii) $\lambda \cdot (v + w) = \lambda \cdot v + \lambda \cdot w$
- iii) $\lambda \cdot (\mu \cdot v) = (\lambda \cdot \mu) \cdot v$
- iv) $1 \cdot v = v$

Remarks:

- The vector space axioms allow for an abstract study and serve as an interface to the developed theory.
For example, this is important for the study of linear equations, where the sought after solutions are functions (e.g., differential or integral equations). We then look for solutions in particular function spaces (typically infinite-dimensional which we approximate with finite-dimensional ones on the computer).
- Often one equips vector spaces with additional structure: Norm (abstract notion of length), inner product (relates to angles and orthogonality), topology (relates to limits, continuity and connectedness),...
→ Below we will introduce inner product spaces (a preliminary stage to so-called Hilbert Spaces)

Example 7.6

- (i) \mathbb{R} , \mathbb{C} , \mathbb{R}^n , C^n , $\mathbb{R}^{m \times n}$

Let us verify the axioms for $\mathbb{R}^{m \times n}$. We have defined matrix sum $+$ and scaling \cdot .

(VR1) $(\mathbb{R}^{m \times n}, +)$ is a commutative group:

...

(VR2) Recall the compatibility properties from Lemma ??:

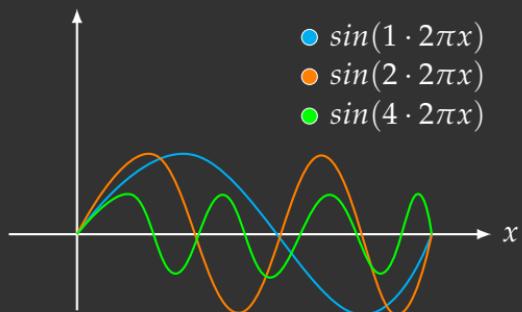
Let $A, B \in \mathbb{R}^{m \times n}$ and $r, s \in \mathbb{R}$. Then

- i) $(r + s) \cdot A = r \cdot A + s \cdot A$
- ii) $r \cdot (A + B) = r \cdot A + r \cdot B$
- iii) $(r \cdot s) \cdot A = r \cdot (s \cdot A)$
- iv) $1 \cdot A = A$

(ii) Let $V := \{\rho \mid \rho : [0, 1] \rightarrow \mathbb{R}\}$ and define

$$(\lambda \cdot \rho)(x) := \lambda \cdot \rho_2(x), \quad (\rho_1 + \rho_2)(x) := \rho_1(x) + \rho_2(x)$$

Functional analysis deals with infinite dimensional vector spaces of functions and generalizes/extends results from linear algebra.



(iii) Gray-scale images of size 1024×1024 :

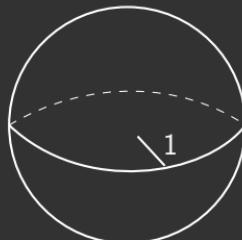
$$\{A \in \mathbb{R}^{1024 \times 1024} \mid a_{ij} \in [0, 1]\}$$

is only a subset of a vector space, not a vector space as such. It is a convex set though.

(iv) The two-dimensional sphere in \mathbb{R}^3 is defined by

$$S^2 = \{x \in \mathbb{R}^3 \mid \|x\| = 1\}$$

for some norm $\|\cdot\|$. For the Euclidean norm it looks like this:



This is not a vector space (curvature prevents a simple summation of two elements), but a so-called **manifold**.

(v) Let $n \in \mathbb{N}$ and $P_n(\mathbb{R})$ be the set of all polynomials of degree $\leq n$ on \mathbb{R} , i.e., the set $P_n(\mathbb{R})$ contains all functions $p : \mathbb{R} \rightarrow \mathbb{R}$ of the form

$$p(x) = \sum_{k=0}^n \alpha_k x^k$$

for some $\alpha_0, \dots, \alpha_n \in \mathbb{R}$. We define a summation and scalar multiplication:

$$\begin{aligned} + &: P_n(\mathbb{R}) \times P_n(\mathbb{R}) \rightarrow P_n(\mathbb{R}), \quad (p+q)(x) := p(x) + q(x), \\ \cdot &: \mathbb{R} \times P_n(\mathbb{R}) \rightarrow P_n(\mathbb{R}), \quad (r \cdot p)(x) := r \cdot p(x). \end{aligned}$$

Monomials $q_k : \mathbb{R} \rightarrow \mathbb{R}$, $x \mapsto x^k$ form a basis of this $(n+1)$ -dimensional vector space.

7.2 Revisit: Linear Combination, Linear Independence, Basis

Based on the more abstract functions $+$ and \cdot we can generally define:

Definition 7.7 Let V be a vector space over the field \mathbb{F} and $v_1, \dots, v_r \in V$. Then, we define

a) **Linear combination:**

$$\sum_{j=1}^r \lambda_j v_j \in V, \quad \lambda_j \in \mathbb{F}$$

b) **Span (set of all linear combinations):**

$$\text{span}(v_1, \dots, v_r) := \left\{ \sum_{j=1}^r \lambda_j v_j : \lambda_j \in \mathbb{F}, j = 1, \dots, r \right\} \in V$$

d) The vectors v_1, \dots, v_r are called **linearly independent**, if

$$\sum_{j=1}^r \lambda_j v_j = 0 \Rightarrow \lambda_j = 0, \forall j = 1, \dots, r$$

e) The vectors v_1, \dots, v_r are called **basis of V** , if

- i) v_1, \dots, v_r are linearly independent,
- ii) $\text{span}(v_1, \dots, v_r) = V$.

With the same proof as for \mathbb{F}^n we can show:

Corollary 7.8 For vectors $v_1, \dots, v_r \in V$ the following statements are equivalent:

- i) v_1, \dots, v_r are linearly independent
- ii) every vector $v \in \text{span}(v_1, \dots, v_r)$ can be uniquely linearly combined from the set $\{v_1, \dots, v_r\}$.
- iii) None of v_i for $i = 1, \dots, r$ can be written as a linear combination of the other.

Remark: Note that these notions coincide with the ones from the linear algebra section. However, now "vectors" are elements from any vector space V and could thus be vectors in the discrete sense, or matrices, or functions,...

Example 7.9

Let $V := \mathbb{R}^{2 \times 3}$, then a basis of length 6 is given by

$$\left\{ \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}, \dots, \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix} \right\}$$

Independent: ✓

Generating:

$$\begin{pmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \end{pmatrix} = a_{11} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + a_{12} \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 0 \end{pmatrix} + a_{13} \begin{pmatrix} 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix} \\ + a_{21} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix} + a_{22} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} + a_{23} \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

The basis is of length 6 and thus $\dim(V) = 6 (= 2 \cdot 3)$.

7.3 Linear functions: kernel, image, matrix representation

Definition 7.10 (Linear function) Let V, W be two vector spaces over \mathbb{F} . Then a function $f : V \rightarrow W$ is called an \mathbb{F} -linear function, if

$$f(\lambda v_1 +_V v_2) = \lambda f(v_1) +_W f(v_2) \quad \forall v_1, v_2 \in V, \lambda \in \mathbb{F}.$$

The set of all linear functions is denoted by $\text{Hom}_{\mathbb{F}}(V, W)$ (homomorphisms).

For $f \in \text{Hom}_{\mathbb{F}}(V, W)$ we define the **kernel** $\ker(f)$ and the **image** $\text{Im}(f)$ as

$$\ker(f) := \{v \in V : f(v) = 0\} \subset V,$$

$$\text{Im}(f) := \{f(v) \in W : v \in V\} \subset W.$$

Example 7.11

(i) $0 : V \rightarrow W, v \mapsto 0 \in W$

Check: $0(\lambda v_1 + v_2) = 0 = 0 + 0 = \lambda 0(v_1) + 0(v_2) \quad \forall v_1, v_2 \in V, \lambda \in \mathbb{F}.$

(ii) $\text{id} : V \rightarrow V, v \mapsto v$

Check: $\text{id}(\lambda v_1 + v_2) = \lambda v_1 + v_2 = \lambda \text{id}(v_1) + \text{id}(v_2) \quad \forall v_1, v_2 \in V, \lambda \in \mathbb{F}.$

(iii) If $\{v_1, \dots, v_n\}$ is a basis of V and $\lambda \in \mathbb{F}^n$ the coordinate representation of $v \in V$, i.e., $v = \sum_{i=1}^n \lambda_i v_i$.
Then, the function

$$\pi_i : V \rightarrow \mathbb{F}, \quad v \mapsto \lambda_i$$

is linear.

(iv) The derivative $\frac{d}{dx}$ and the integral \int operators are linear functions.

Matrix Representation of Linear Mappings

Next we show that for finite-dimensional vector spaces V and W , say $\dim(V) = n$ and $\dim(W) = m$, the set of all linear functions from V to W is equivalent to the set of all $m \times n$ matrices.

Introductory example:

Let us consider polynomials of degree no higher than 2, i.e., $\mathcal{P}_2(\mathbb{R})$. Then an example of a linear function from $\mathcal{P}_2(\mathbb{R})$ ($n = 3$) to $\mathcal{P}_1(\mathbb{R})$ ($m = 2$) is given by the derivative $f(\cdot) := \frac{d}{dx}(\cdot)$.

Examples:

- $p(x) = x + 2x^2 \quad \simeq (0, 1, 2)$
 $\frac{d}{dx}p(x) = 1 + 4x \quad \simeq (1, 4)$
- $p(x) = 1 + 3x^2 \quad \simeq (1, 0, 3)$
 $\frac{d}{dx}p(x) = 6x \quad \simeq (0, 6)$

In terms of the coordinates, the derivative $\frac{d}{dx}$ can be represented by the matrix

$$\begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 2 \end{pmatrix}.$$

[ex:commutative diagram]

Remark 7.12

- The matrix $\mathcal{M}_{\{w_1, \dots, w_m\}}^{\{v_1, \dots, v_n\}}(f)$ is sometimes called *transformation matrix* (in German: *Darstellungsmatrix*).
- It is the matrix representation of f under the given bases and it tells us how to transform the coordinates!
- Also, it establishes a one-to-one relation between $\text{Hom}_{\mathbb{F}}(V, W)$ and $\mathbb{F}^{m \times n}$, i.e.,

$$\text{Hom}_{\mathbb{F}}(V, W) \simeq \mathbb{F}^{m \times n}.$$

Example 7.13

- i) Exercise: Let $f \in \text{Hom}_{\mathbb{F}}(\mathbb{F}, \mathbb{F})$ and $v_1 \neq 0 \neq w_1$ two real numbers, each forming a basis of \mathbb{F} .
- ii) Let $f \in \text{Hom}_{\mathbb{F}}(\mathbb{F}^n, \mathbb{F}^m)$ and consider the two bases $V = (v_1, \dots, v_n) \in \text{GL}_n(\mathbb{F})$, and $W = (w_1, \dots, w_m) \in \text{GL}_m(\mathbb{F})$. Note that the basis vectors are now vectors in our sense so far and we can now stack them into matrices. Also, for simplicity we write

$$\mathcal{M}_W^V(f) := \mathcal{M}_{\{w_1, \dots, w_m\}}^{\{v_1, \dots, v_n\}}(f).$$

We observe

$$f(v_j) = \sum_{j=1}^m a_{ij} w_j \Leftrightarrow (a_{ij})_i = W^{-1} f(v_j),$$

so that the representing matrix of f is given by

$$\mathcal{M}_W^V(f) := W^{-1}(f(v_1), \dots, f(v_n)) \in \mathbb{F}^{m \times n}$$

and

$$f(v) = f(VV^{-1}v) = W\mathcal{M}_W^V(f)V^{-1}v.$$

[ex: Draw commutative diagram.]

iia) Take for example $f(v) := Av$ for some $A \in \mathbb{F}^{m \times n}$, so that $f \in \text{Hom}_{\mathbb{F}}(\mathbb{F}^n, \mathbb{F}^m)$. Then

$$\mathcal{M}_I^I(f) = \dots = A$$

and

$$\mathcal{M}_W^V(f) = \dots = W^{-1}AV$$

iib) In particular, if $m = n$ (so we can choose the same basis for $V = W = \mathbb{F}^n$), we observe

$$\mathcal{M}_I^I(f) = \dots = A$$

and

$$\mathcal{M}_V^V(f) = \dots = V^{-1}AV.$$

Observations:

- $\mathcal{M}_I^I(f)$ and $\mathcal{M}_V^V(f)$ are similar. Hence, they have the same eigenvalues.
- The matrix representation depends on the chosen basis, but the somewhat deeper properties (eigenvalues,...) of the linear map as such are unchanged.
- This leads to the idea of searching for a particular basis in order to get a matrix representation, which reveals the “essence” of the respective linear function. If the eigenvectors form a basis then they would be a good choice: In this case the matrix representation is diagonal having precisely the eigenvalues on its diagonal.

iii) Consider

$$\text{Hom}_{\mathbb{R}}(\mathbb{R}^n, \mathbb{R}) = \{f: \mathbb{R}^n \rightarrow \mathbb{R} : f \text{ linear}\} \quad (\text{dual space of } \mathbb{R}^n).$$

Let $V = (v_1, \dots, v_n) \in \text{GL}_n(\mathbb{R})$ and $\{1\}$ be a bases for V and \mathbb{R} , respectively. Then for $f \in \text{Hom}_{\mathbb{R}}(\mathbb{R}^n, \mathbb{R})$ obviously $f(v_j) = f(v_j) \cdot 1$, so that

$$\mathcal{M}_I^V(f) = \mathcal{M}_{\{1\}}^{\{v_1, \dots, v_n\}}(f) = (f(v_1), \dots, f(v_n)) \in \mathbb{R}^{1 \times n}$$

is simply a row vector.

For $v = VV^{-1}v =: V\lambda \in \mathbb{R}^n$ we have

$$f(v) = \sum_{j=1}^n \lambda_j f(v_j) = \mathcal{M}_{\{1\}}^{\{v_1, \dots, v_n\}}(f) \cdot \lambda = \mathcal{M}_{\{1\}}^{\{v_1, \dots, v_n\}}(f) V^{-1} \cdot v = \left(\left(\mathcal{M}_{\{1\}}^{\{v_1, \dots, v_n\}}(f) V^{-1} \right)^{\top}, v \right)_2.$$

Important observations/remarks

- In words: The column vector $v_f := \left(\mathcal{M}_{\{1\}}^{\{v_1, \dots, v_n\}}(f) V^{-1} \right)^{\top}$ represents the linear function f in the standard inner product

$$f(\cdot) = (v_f, \cdot)_2.$$

This is the finite-dimensional “light version” of the Riesz representation theorem.

- If we choose the standard basis $V = I$, then this vector is simply

$$\mathcal{M}_I^I(f)^{\top} = \begin{pmatrix} f(v_1) \\ \vdots \\ f(v_n) \end{pmatrix} \in \mathbb{R}^n.$$

- In the next section we consider general inner products $(\cdot, \cdot)_A$ on \mathbb{R}^n and how this effects the representing vector v_f :

$$f(\cdot) = (v_f^A, \cdot)_A = (v_f, \cdot)_2.$$

- When considering the derivative $DF(x): \mathbb{R}^n \rightarrow \mathbb{R}$ as a linear mapping we will call the vector $\mathcal{M}_I^I(DF(x))^{\top}$ the gradient of F at point x (represented in the standard basis and standard inner product).

7.4 Inner Product Spaces

We now add more structure to a vector space: We equip it with an inner product.

Definition 7.14 Let V be a vector space over \mathbb{F} .

- A mapping $(\cdot, \cdot): V \times V \rightarrow \mathbb{F}$ is called **inner product** on \mathbb{F}^n if it satisfies:
 - i) **Hermitian:** $\forall x, y \in V : (x, y) = \overline{(y, x)}$,
 - ii) **Linear in its second argument:** $\forall x, y_1, y_2 \in V, \lambda \in \mathbb{F} : (x, y_1 + \lambda y_2) = (x, y_1) + \lambda(x, y_2)$,
 - iii) **Positive definite:** $\forall x \in V \setminus \{0\} : (x, x) > 0$.
- We call $(V, (\cdot, \cdot))$ an **Euclidean vector space or inner product space**.

For simplicity we now stick to $V = \mathbb{R}^n$. We can show the following characterization:

Theorem 7.15 Let $(\cdot, \cdot): \mathbb{R}^n \times \mathbb{R}^n \rightarrow \mathbb{R}$, then

$$(\cdot, \cdot) \text{ inner product on } \mathbb{R}^n \Leftrightarrow \exists A \in \mathbb{R}_{spd}^{n \times n} \forall x, y \in \mathbb{R}^n : (x, y) := (x, y)_A := (x, Ay)_2.$$

In words: There is a one-to-one relation between all inner products on \mathbb{R}^n and all symmetric and positive definite matrices in $\mathbb{R}^{n \times n}$. The proof is constructive and reveals that the entries of A are given by

$$a_{ij} := (e_i, e_j)$$

where e_j denote the standard basis vectors.

Final note:

Let us again consider $\text{Hom}_{\mathbb{R}}(\mathbb{R}^n, \mathbb{R})$ and now a general inner product $(\cdot, \cdot)_A$ on \mathbb{R}^n for some spd matrix $A \in \mathbb{R}^{n \times n}$.

Question

For $f \in \text{Hom}_{\mathbb{R}}(\mathbb{R}^n, \mathbb{R})$ we know $f: \mathbb{R}^n \rightarrow \mathbb{R}$ is linear. On the other hand $(v, \cdot)_A: \mathbb{R}^n \rightarrow \mathbb{R}$ is linear for a fixed vector $v \in \mathbb{R}^n$ and inner product $(\cdot, \cdot)_A$, i.e., $(v, \cdot)_A \in \text{Hom}_{\mathbb{R}}(\mathbb{R}^n, \mathbb{R})$. Thus it is natural to ask whether there is a one-to-one relation between $\text{Hom}_{\mathbb{R}}(\mathbb{R}^n, \mathbb{R})$ and \mathbb{R}^n , i.e., can we find a unique $v_f^A \in \mathbb{R}^n$ for $f \in \text{Hom}_{\mathbb{R}}(\mathbb{R}^n, \mathbb{R})$ so that $f(\cdot) = (v_f^A, \cdot)_A$?

Yes we can: In fact, define $v_f := v_f^I := (\mathcal{M}_I^I(f))^\top$, then using the findings from above and the properties of A we get

$$f(v) = (v_f, v)_2 = v_f^\top v = v_f^\top (A^{-1}A)v = v_f^\top (A^{-1})^\top A v = (A^{-1}v_f, Av)_2 = (A^{-1}v_f, v)_A.$$

In words:

- Fixing to the standard inner product $A = I$, we find

$$v_f^I = (\mathcal{M}_I^I(f))^\top$$

- Changing to a general inner product, we find

$$v_f^A = A^{-1}v_f^I$$

The important relation to Data Science/Optimization

- The gradient (times (-1)) of a function determines a descent direction. Moving in this direction will minimize the function
- The gradient is precisely the vector representing the derivative of a function.
- You will learn how to accelerate the gradient method by representing it in another inner product, e.g., the one induced by the Hessian $A = H_f(x)$ (this will give you Newton type method!).

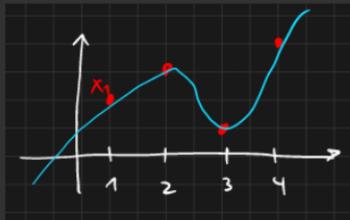
Calculus

8 Nonlinear Aspects

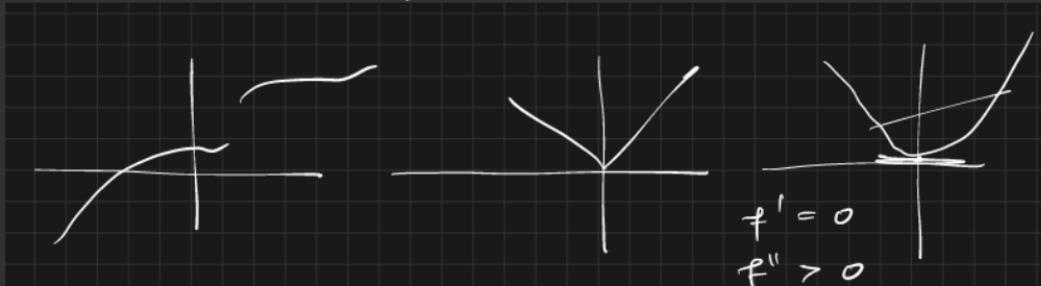
We will touch upon the following topics:

- continuous and differentiable functions
- partial derivatives, gradient, Jacobian
- (chain rule)
- In exercise: Taylor approximation and Newton's method

Until now we have worked with "discrete objects", say $x \in \mathbb{R}^n$, $\{1, \dots, n\} \rightarrow \mathbb{R}$, $i \mapsto x_i$



Now, vectors become functions $f : \mathbb{R} \rightarrow \mathbb{R}$



8.1 Motivation

Let us first recall the definition of a linear function. Consider a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$, then

$$f \text{ linear } \stackrel{\text{Def}}{\Leftrightarrow} \forall x, y \in \mathbb{R}^n, \lambda \in \mathbb{R} : f(\lambda \cdot x + y) = \lambda \cdot f(x) + f(y).$$

The prototype of a linear function between finite dimensional spaces is the matrix–vector product, more precisely,

$$A \in \mathbb{R}^{m \times n}, f_A(x) := Ax.$$

We say f is **nonlinear**, if it is not linear.

Nonlinear function may extend our modeling choice significantly and may help to explain complicated relations, such as

$$\begin{array}{ccc} z_i & \rightarrow & y_i \\ \in \mathbb{R}^p & & \in \mathbb{R}^q, i = 1, \dots, m. \\ [\text{image}] & & [\text{feature}] \end{array}$$

Until now, we have consider models with *linear* dependency of the parameters:

$$f_x(z) = \sum_{k=1}^n x_k \cdot f_k(z) \approx y.$$

We determined the parameters $x = (x_k)_k$ by solving a (potentially regularized) least squares problem of the form

$$\min_x L(x; (z_i, y_i)) + R(x), \quad \left(\text{e.g., Ridge Regression } R(x) := \frac{\delta}{2} \|x\|_2^2 \right),$$

where the cost function has the form

$$\sum_{i=1}^m \|f_x(z_i) - y_i\|_2^2 = \|A_z x - y\|_2^2 =: L(x, (z_i, y_i)).$$

The specialty of this kind of minimization problem is that we can solve it via the normal equation, which is a *linear* equation.

Now let us consider a **nonlinear model** (e.g. Neural Network); more precisely, nonlinear with respect to the sought-after parameters. More specifically, let us for example consider a model of the form

$$f_x(z) = (f_M \circ \dots \circ f_1)(z) = f_M(f_{M-1}(f \dots (f_1(z)) \dots))$$

where the building blocks f_k , also called **layers**, are given by

$$f_k: \mathbb{R}^p \rightarrow [0, +\infty)^q, \quad f_k(z) := (A_k z + b_k)_+ \quad (\text{applied element-wise}),$$

with

$$\mathbb{R} \rightarrow [0, +\infty), \quad w_+ := \begin{cases} 0 : w < 0 \\ w : \text{else} \end{cases}$$

being the so-called **ReLU function** (Rectified Linear Unit), an example of a so-called **activation function**.

The matrices $A_k \in \mathbb{R}^{q \times p}$ and vectors $b_k \in \mathbb{R}^q$ are the parameters (also called **weights**) that need to be determined. If A_k is dense, the function f_k is called **fully connected layer** and if, e.g., A_k is Toeplitz, then f_k is called **convolutional layer**.

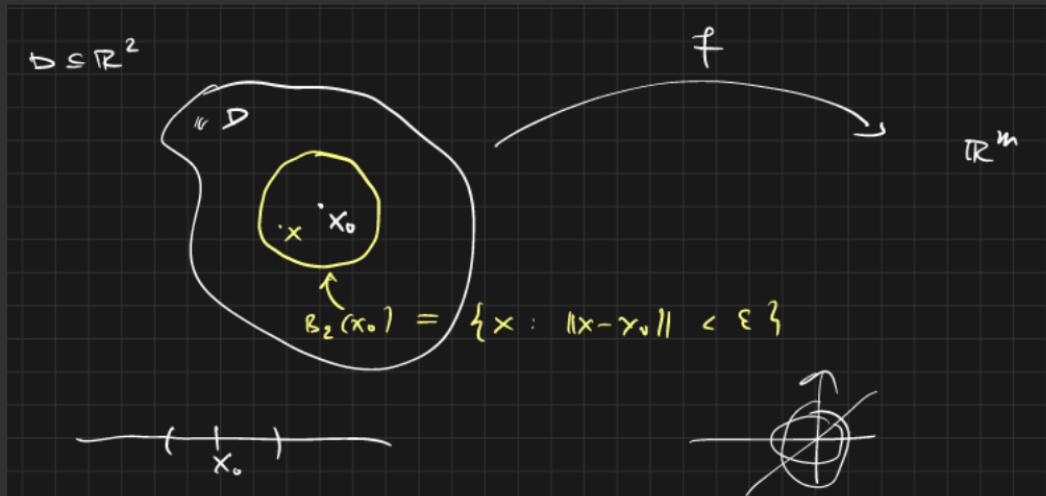
Due to the ReLU function $(\cdot)_+$ the concatenated model f_x is highly nonlinear.

Similarly to the linear case, we aim to find suitable parameters/weights $x := (A_k, b_k)_k$ that best describe the model with respect to a certain cost function:

$$\min_{x:=(A_k, b_k)_k} L(x; (z_i, y_i)) + R(x) =: F(x) \quad (\leftarrow F \text{ highly nonlinear})$$

Before we continue with some standard definitions from calculus, a preliminary remark:

The concepts of continuity and differentiability in the context of a function $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ are "local" concepts, i.e., they are required to hold in a small neighborhood of a point $x_0 \in \mathbb{R}^n$.



8.2 Continuity and Differentiability

In the following we consider neighborhoods of the form $B_\varepsilon(x_0) := \{x \in \mathbb{R}^n : \|x - x_0\| < \varepsilon\}$.

Definition 8.1 (Continuous and differentiable function)

Let $D \subseteq \mathbb{R}^n$, $f : D \rightarrow \mathbb{R}^m$ and $x_0 \in D$ with $B_\varepsilon(x_0) \subseteq D$ for some $\varepsilon > 0$. Then

i) f is called **continuous** at x_0 , if

$$\lim_{n \rightarrow 0} \|f(x_n) - f(x_0)\|_2 = 0$$

for all sequences $(x_n)_{n \in \mathbb{N}} \subseteq B_\varepsilon(x_0)$ for which $x_n \rightarrow x_0$.

ii) f is called **differentiable** at x_0 , if there is a linear mapping $A : \mathbb{R}^n \rightarrow \mathbb{R}^m$ such that

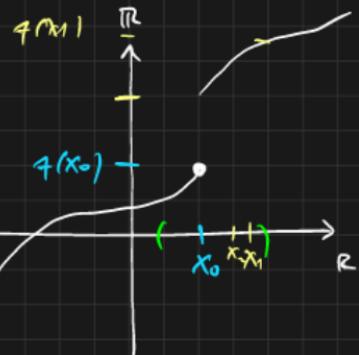
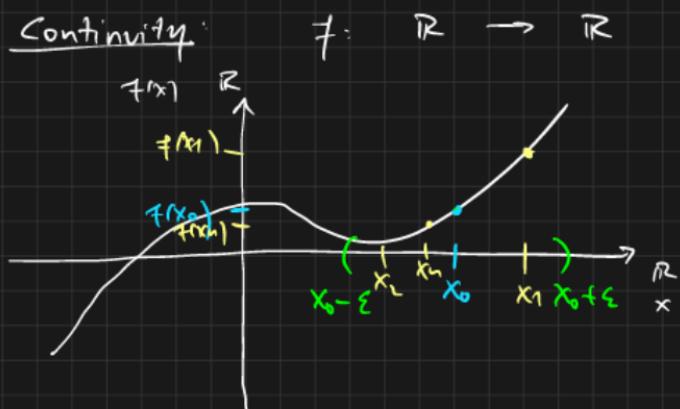
$$\lim_{n \rightarrow \infty} \frac{\|(f(x_0) + Ah_n) - f(x_0 + h_n)\|}{\|h_n\|} = 0$$

for all sequences $(h_n)_n$ with $x_0 + h_n \subseteq B_\varepsilon(x_0)$, $\lim_{n \rightarrow \infty} \|h_n\| \rightarrow 0$.

Since the linear function A depends on f and x_0 , we denote it as $Df(x_0) := A$ and call it (Fréchet) derivative.

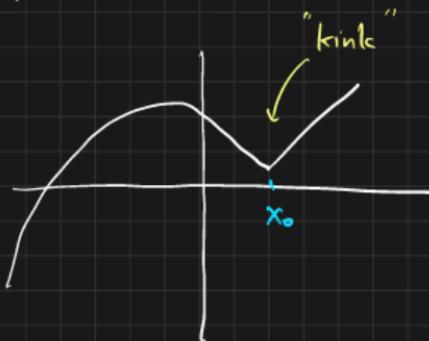
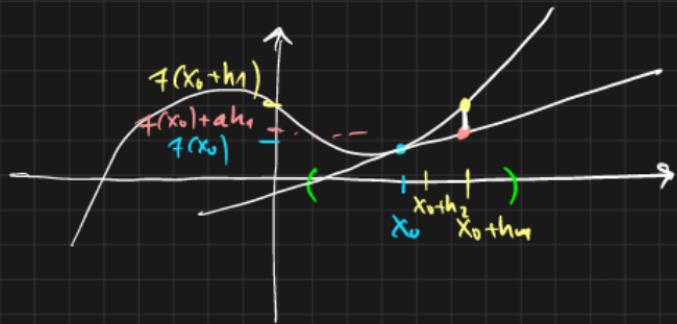
If f is continuous/differentiable at any point $x_0 \in D$, we call f simply continuous/differentiable.

Continuity



Differentiable

$$f: \mathbb{R} \rightarrow \mathbb{R}, Df(x_0), \frac{d}{dh} | f(x_0) + a \cdot h - f(x_0 + h) |$$



Examples: Continuity

i) $f : \mathbb{R} \rightarrow \mathbb{R}, x \mapsto |x| = \begin{cases} x & x \geq 0 \\ -x & x < 0 \end{cases}$

Let $x_0 \in \mathbb{R}, (x_n)_{n \in \mathbb{N}}, x_n \xrightarrow{n \rightarrow \infty} x_0$, then

$$0 \leq |f(x_n) - f(x_0)| = ||x_n| - |x_0|| \leq |x_n - x_0| \xrightarrow{n \rightarrow 0} 0$$

$\Rightarrow f$ is continuous.

ii) $f : \mathbb{R} \rightarrow \mathbb{R}, x \mapsto x^2$

Let $x_0 \in \mathbb{R}, x_n \rightarrow x_0$, then

$$|f(x_n) - f(x_0)| = |x_n^2 - x_0^2| = |(x_n - x_0)(x_n + x_0)| = \underbrace{|x_n - x_0|}_{\rightarrow 0} \underbrace{|x_n + x_0|}_{\rightarrow 2x_0} \xrightarrow{n \rightarrow \infty} 0$$

$\Rightarrow f$ is continuous.

iii) $f : \mathbb{R} \rightarrow \mathbb{R}, f(x) := \begin{cases} 1 & x > 0 \\ -1 & x \leq 0 \end{cases}$

Let $x_0 = 0, x_n \rightarrow 0^+$, then

$$|f(x_n) - f(x_0)| = |1 - (-1)| = 2 \not\rightarrow 0$$

$\Rightarrow f$ is not continuous.

Examples: Differentiability

i) $f : \mathbb{R} \rightarrow \mathbb{R}, x \mapsto ax, a \in \mathbb{R}$

Let us consider the surrogate $Df(x_0)(h) := ah$ and a sequence $h_n \rightarrow 0$. Then

$$\frac{1}{|h_n|} |f(x_0) + Df(x_0)h_n - f(x_0 + h_n)| = \frac{1}{|h_n|} |ax_0 + ah_n - a(x_0 + h_n)| = 0 \xrightarrow{n \rightarrow \infty} 0$$

$\Rightarrow f$ is differentiable.

ii) $f : \mathbb{R}^n \rightarrow \mathbb{R}^m, x \mapsto Ax, A \in \mathbb{R}^{m \times n}$

Let us consider the surrogate $Df(x_0)(h) := Ah$ and a sequence $h_n \rightarrow 0$. Then

$$\frac{1}{|h_n|} |f(x_0) + Df(x_0)h_n - f(x_0 + h_n)| = \frac{1}{|h_n|} |Ax_0 + Ah_n - A(x_0 + h_n)| = 0 \xrightarrow{n \rightarrow \infty} 0$$

$\Rightarrow f$ is differentiable.

iii) $f : \mathbb{R} \rightarrow \mathbb{R}, x \mapsto |x|$

f is **not** differentiable at $x_0 = 0$.

Remark: How can we identify continuous/differentiable functions?

- Many elementary functions (polynomials, trigonometric functions, exponential function,...) and operations ("+", "·", ...) to combine such elementary functions are continuous/differentiable.
- The concatenation of such functions is also continuous/differentiable!
- Examples:

- monomial x^k and polynomial (=linear combination) $p(x) = \sum_{j=0}^m a_j x^j$
- exponential function e^x and sine function $\sin(x) = \frac{1}{2i}(e^{ix} - e^{-ix})$

We will show in the exercise that differentiability is a stronger requirement than continuity:

Theorem 8.2 *Every differentiable function is also continuous.*

Next, we introduce the directional derivative which often serves as a good starting point to find the (Fréchet) derivative of a function (especially in complex and confusing situations):

Definition 8.3 (Directional derivative) We assume that $f : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is (Fréchet-) differentiable at $x_0 \in \mathbb{R}^n$ with derivative $Df(x_0)$. For a $v \in \mathbb{R}^n$, the limit

$$Gf(x_0)(v) := \lim_{t \rightarrow 0^+} \frac{f(x_0 + tv) - f(x_0)}{t}$$

exists and it concides with the Fréchet derivative, i.e., $Gf(x_0)(v) = Df(x_0)(v)$.

We call $Gf(x_0)(v)$ the **directional derivative** at x_0 in the direction v . (Gâteaux derivative)

Remark:

The Gâteaux derivative may exist, even if f is not Fréchet differentiable (e.g. $x \mapsto |x|$, $x_0 = 0$).

Examples:

i) $f : \mathbb{R} \rightarrow \mathbb{R}$, $x \mapsto |x|$, $x_0 = 0$ (not Fréchet-differentiable)

$$\begin{aligned} \text{a)} \ v \geq 0: \ Gf(x_0)(v) &= \lim_{t \rightarrow 0^+} \frac{1}{t}(f(x_0 + tv) - f(x_0)) = \lim_{t \rightarrow 0^+} \frac{1}{t}(tv) = 1 \cdot v \\ \text{b)} \ v < 0: \ Gf(x_0)(v) &= \lim_{t \rightarrow 0^+} \underbrace{\frac{1}{t}(f(x_0 + tv) - f(x_0))}_{=-tv} = (-1) \cdot v \end{aligned}$$

ii) $f : \mathbb{R}^n \rightarrow \mathbb{R}$, $x \mapsto \|x\|_2^2 = x^T x$, $v \in \mathbb{R}^n$, $x_0 \in \mathbb{R}^n$

$$\begin{aligned} Gf(x_0)(v) &= \lim_{t \rightarrow 0^+} \frac{f(x_0 + tv) - f(x_0)}{t} \\ &= \lim_{t \rightarrow 0^+} \left(\frac{(x_0 + tv)^T (x_0 + tv)}{x_0^T x_0 + 2tx_0^T v + t^2 v^T v} - x_0^T x_0 \right) \frac{1}{t} \\ &= (2x_0)^T v \end{aligned}$$

Consider $v = \sum_{j=1}^n v_j e_j$, where e_1, \dots, e_n denote the standard basis in \mathbb{R}^n , then

$$Df(x_0)(v) = \sum_{j=1}^n v_j \underbrace{Df(x_0)(e_j)}_{\substack{\mathbb{R}^n \rightarrow \mathbb{R}^m \\ \in \mathbb{R}^m}}$$

Definition 8.4 (Partial derivative) Let $f : D \rightarrow \mathbb{R}^m$, $D \subseteq \mathbb{R}^n$ be (Fréchet-)differentiable in $x_0 \in D$. We define the so-called **partial derivatives** of f at x_0 with respect to the j -th variable by:

$$\frac{\partial}{\partial x_j} f(x_0) := Df(x_0)(e_j),$$

where e_j is the j -th standard basis vector.

Now again with $v = \sum_{j=1}^n v_j e_j$ we find

$$\begin{aligned} Df(x_0)(v) &= \sum_{j=1}^n v_j Df(x_0)(e_j) \\ &= \begin{pmatrix} | & & | \\ Df(x_0)(e_1) & \cdots & Df(x_0)(e_n) \\ | & & | \end{pmatrix} \begin{pmatrix} v_1 \\ \vdots \\ v_n \end{pmatrix} \\ &= \begin{pmatrix} | \\ \frac{\partial}{\partial x_1} f(x_0) \\ | & \cdots & | \\ \frac{\partial}{\partial x_n} f(x_0) \end{pmatrix} v \\ &= \underbrace{J_f(x_0)}_{\in \mathbb{R}^{m \times n}} \cdot v \\ f : \mathbb{R}^n &\rightarrow \mathbb{R}^m, f(x) = \begin{pmatrix} f_1(x) \\ \vdots \\ f_m(x) \end{pmatrix}, f_i : \mathbb{R}^n \rightarrow \mathbb{R} \end{aligned}$$

Since $Df(x_0) : \mathbb{R}^n \rightarrow \mathbb{R}^m$ is linear it can be represented by a matrix:

Lemma 8.5 (Jacobian) Let $f : \mathbb{R}^n \supset D \rightarrow \mathbb{R}^m$ be differentiable at $x_0 \in D$ with derivative $Df(x_0) : \mathbb{R}^n \rightarrow \mathbb{R}^m$. Then the so-called **Jacobian matrix**

$$J_f(x_0) := \mathcal{M}_I^I(Df(x_0)) = \begin{pmatrix} \frac{\partial f_1}{\partial x_1}(x_0) & \cdots & \frac{\partial f_1}{\partial x_n}(x_0) \\ \vdots & \ddots & \vdots \\ \frac{\partial f_m}{\partial x_1}(x_0) & \cdots & \frac{\partial f_m}{\partial x_n}(x_0) \end{pmatrix} \in \mathbb{R}^{m \times n}$$

is the matrix representation of $Df(x_0)$ with respect to the standard bases in \mathbb{R}^n and \mathbb{R}^m .

In the special case, that the Jacobian matrix is just one row we give it a special name:

Definition 8.6 (Gradient) Let $f : \mathbb{R}^n \supset D \rightarrow \mathbb{R}$ be differentiable at $x_0 \in D$, then

$$J_f(x_0)^T = \begin{pmatrix} \frac{\partial f}{\partial x_1}(x_0) \\ \vdots \\ \frac{\partial f}{\partial x_n}(x_0) \end{pmatrix} =: \nabla f(x_0)$$

is called the **gradient of f** at $x_0 \in D$.

Example

Let us again consider $f : \mathbb{R}^n \rightarrow \mathbb{R}$ with

$$x \mapsto x^T x = \sum_{i=1}^n x_i^2 = x_1^2 + x_2^2 + \cdots + x_n^2.$$

Then

$$\frac{\partial f}{\partial x_i}(x) = 2x_i$$

$$\nabla f(x) = 2 \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} = 2x$$

$$Df(x)(v) = (2x)^T v$$

$$J_f(x) \cdot v = \nabla f(x)^T \cdot v = (2x)^T v$$

8.3 Solving Nonlinear Equations: Taylor Approximation and Newton's Method

The next result is on the approximation quality of the derivative:

Lemma 8.7 (Taylor approximation) Let $f : \mathbb{R}^n \supset B_\varepsilon(\hat{x}) \rightarrow \mathbb{R}^n$ be differentiable at \hat{x} with some $\varepsilon > 0$. Assume further that there is a (Lipschitz) constant $L \geq 0$ such that the Jacobian J_f satisfies

$$\|J_f(y) - J_f(x)\| \leq L\|y - x\|, \quad \forall x, y \in B_\varepsilon(\hat{x}). \quad (18)$$

Then, there holds

$$\|f(y) - [f(x) + J_f(x)(y - x)]\| \leq \frac{L}{2}\|y - x\|^2, \quad \forall x, y \in B_\varepsilon(\hat{x})$$

which we rephrase with the notation:

$$f(y) = f(x) + J_f(x)(y - x) + \mathcal{O}(\|y - x\|^2).$$

Let us apply Taylor approximation to solve nonlinear systems: The idea is to locally approximate the nonlinear function by its linear derivative and then solve many linear systems.

- Situation: Consider for a potentially nonlinear function $f : \mathbb{R}^n \rightarrow \mathbb{R}^n$ and the nonlinear system $f(\hat{x}) = 0$
- Aim: Determine the solution \hat{x} (iteratively/numerically)
- Idea: Define an iterative scheme $x^{k+1} := x^k + \Delta x^k$ where the increment is derived as follows:

$$\begin{aligned} 0 &\stackrel{!}{=} f(x^{k+1}) = f(x^k + \Delta x^k) \approx f(x^k) + J_f(x^k)\Delta x^k \quad (\leadsto \text{solve for } \Delta x^k) \\ \Leftrightarrow J_f(x^k) \cdot \Delta x^k &= -f(x^k) \quad (\text{linear equation}) \\ \Leftrightarrow \Delta x^k &= -J_f(x^k)^{-1}f(x^k) \quad (\text{invertibility of the derivative at each } x_k \text{ assumed!}) \\ x^k &\rightarrow \hat{x} \end{aligned}$$

One can show the following convergence result of this approach:

Theorem 8.8 (simplified Newton-Kantorovich) Let $f : \mathbb{R}^n \supset B_\varepsilon(\hat{x}) \rightarrow \mathbb{R}^n$ be differentiable with invertible derivative for some $\varepsilon > 0$ and $f(\hat{x}) = 0$. Assume the Lipschitz condition (18) and the existence of an upper bound $\|J_f(x)^{-1}\| < M$ for some $M < \infty$ and for all $x \in B_\varepsilon(\hat{x})$. Then, the Newton iteration

$$x^{k+1} := x^k + \Delta x^k, \quad \text{where } \Delta x^k \text{ solves } f(x^k) + J_f(x^k)\Delta x^k = 0$$

converges quadratically to \hat{x} , provided x^1 is chosen sufficiently close to \hat{x} , i.e.

$$\|x^{k+1} - \hat{x}\| \leq c\|x^k - \hat{x}\|^2, \quad c < \infty.$$

Remark

In many cases, Newton's method does not work right out of the box, because the starting vector x^1 is too far away from the solution. Then, techniques for adaptive step-length reduction (damping, relaxation, line-search) have to be used in order to enforce convergence. Details of these approaches fill multiple books. When Newton's method works, i.e., after an initial damped phase, it gets super fast.

Take-away messages:

- Derivatives → local linear approximation to the function
- Newton's method → solves nonlinear systems by solving many linear problems in each step

8.4 The Chain Rule and Back Propagation

The chain rule lies at the heart of back propagation. It tells us how to compute the derivative of concatenated functions:

Theorem 8.9 (Chain rule) Consider mappings $g : \mathbb{R}^\ell \supset D_g \rightarrow D_f \subset \mathbb{R}^m$ differentiable in $x_0 \in D_g$ with Jacobian $J_g(x_0)$ and $f : \mathbb{R}^m \supset D_f \rightarrow \mathbb{R}^n$, differentiable in $g(x_0) \in D_f$ with Jacobian $J_f(g(x_0))$. Then, the concatenation is differentiable with Jacobian $J_{f \circ g}(x_0)$ and

$$D(f \circ g)(x_0) = Df(g(x_0)) \circ Dg(x_0) \quad \text{and} \quad J_{f \circ g}(x_0) = J_f(g(x_0)) \cdot J_g(x_0).$$

Example 8.10 Let us revisit our regularizer from the imaging example:

Consider $D \in \mathbb{R}^{p \times n}$ and the linear function $g : \mathbb{R}^n \rightarrow \mathbb{R}^p$, $g(x) := Dx$. Then for all $x \in \mathbb{R}^n$ we easily find

$$J_g(x) = D.$$

Also, let $f : \mathbb{R}^p \rightarrow \mathbb{R}$, $f(y) := \frac{1}{2}y^\top y = \frac{1}{2}\|y\|_2^2$, then we have seen above that, for all $y \in \mathbb{R}^p$,

$$J_f(y)^\top = \nabla f(y) = \frac{1}{2}2y = y.$$

Then the concatenation $h := (f \circ g) : \mathbb{R}^n \rightarrow \mathbb{R}$ is given by

$$h(x) = \frac{1}{2}\|Dx\|_2^2$$

with gradient, at $x \in \mathbb{R}^n$, obtained from the chain rule

$$\nabla h(x) = J_h(x)^\top = (J_f(g(x)) \cdot J_g(x))^\top = D^\top \nabla f(g(x)) = D^\top g(x) = D^\top Dx.$$