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Machine learning is the latest in a long line of attempts to distill human knowledge and reasoning into a form that is suitable for constructing machines and engineering automated systems. As machine learning becomes more ubiquitous and its software packages become easier to use, it is natural and desirable that the low-level technical details are abstracted away and hidden from the practitioner. However, this brings with it the danger that a practitioner becomes unaware of the design decisions and, hence, the limits of machine learning algorithms.

The enthusiastic practitioner who is interested to learn more about the magic behind successful machine learning algorithms currently faces a daunting set of pre-requisite knowledge:

- Programming languages and data analysis tools
- Large-scale computation and the associated frameworks
- Mathematics and statistics and how machine learning builds on it

At universities, introductory courses on machine learning tend to spend early parts of the course covering some of these pre-requisites. For historical reasons, courses in machine learning tend to be taught in the computer science department, where students are often trained in the first two areas of knowledge, but not so much in mathematics and statistics.

Current machine learning textbooks primarily focus on machine learning algorithms and methodologies and assume that the reader is competent in mathematics and statistics. Therefore, these books only spend one or two chapters on background mathematics, either at the beginning of the book or as appendices. We have found many people who want to delve into the foundations of basic machine learning methods who struggle with the mathematical knowledge required to read a machine learning textbook. Having taught undergraduate and graduate courses at universities, we find that the gap between high school mathematics and the mathematics level required to read a standard machine learning textbook is too big for many people.

This book brings the mathematical foundations of basic machine learning concepts to the fore and collects the information in a single place so that this skills gap is narrowed or even closed.

Why Another Book on Machine Learning?

Machine learning builds upon the language of mathematics to express concepts that seem intuitively obvious but that are surprisingly difficult to formalize. Once formalized properly, we can gain insights into the task we want to solve. One common complaint of students of mathematics around the globe is that the topics covered seem to have little relevance to practical problems. We believe that machine learning is an obvious and direct motivation for people to learn mathematics.

"Math is linked in the popular mind with phobia and anxiety. You'd think we're discussing spiders." (Strogatz, 2014, page 281) 2

This book is intended to be a guidebook to the vast mathematical literature that forms the foundations of modern machine learning. We motivate the need for mathematical concepts by directly pointing out their usefulness in the context of fundamental machine learning problems. In the interest of keeping the book short, many details and more advanced concepts have been left out. Equipped with the basic concepts presented here, and how they fit into the larger context of machine learning, the reader can find numerous resources for further study, which we provide at the end of the respective chapters. For readers with a mathematical background, this book provides a brief but precisely stated glimpse of machine learning. In contrast to other books that focus on methods and models of machine learning (MacKay, 2003; Bishop, 2006; Alpaydin, 2010; Barber, 2012; Murphy, 2012; Shalev-Shwartz and Ben-David, 2014; Rogers and Girolami, 2016) or programmatic aspects of machine learning (Müller and Guido, 2016; Raschka and Mirjalili, 2017; Chollet and Allaire, 2018), we provide only four representative examples of machine learning algorithms. Instead, we focus on the mathematical concepts behind the models themselves. We hope that readers will be able to gain a deeper understanding of the basic questions in machine learning and connect practical questions arising from the use of machine learning with fundamental choices in the mathematical model.

We do not aim to write a classical machine learning book. Instead, our intention is to provide the mathematical background, applied to four central machine learning problems, to make it easier to read other machine learning textbooks.

Who Is the Target Audience?

As applications of machine learning become widespread in society, we believe that everybody should have some understanding of its underlying principles. This book is written in an academic mathematical style, which enables us to be precise about the concepts behind machine learning. We encourage readers unfamiliar with this seemingly terse style to persevere and to keep the goals of each topic in mind. We sprinkle comments and remarks throughout the text, in the hope that it provides useful guidance with respect to the big picture.

The book assumes the reader to have mathematical knowledge commonly

covered in high school mathematics and physics. For example, the reader should have seen derivatives and integrals before, and geometric vectors in two or three dimensions. Starting from there, we generalize these concepts. Therefore, the target audience of the book includes undergraduate university students, evening learners and learners participating in online machine learning courses.

In analogy to music, there are three types of interaction that people have with machine learning:

Astute Listener The democratization of machine learning by the provision of open-source software, online tutorials and cloud-based tools allows users to not worry about the specifics of pipelines. Users can focus on extracting insights from data using off-the-shelf tools. This enables nontech-savvy domain experts to benefit from machine learning. This is similar to listening to music; the user is able to choose and discern between different types of machine learning, and benefits from it. More experienced users are like music critics, asking important questions about the application of machine learning in society such as ethics, fairness, and privacy of the individual. We hope that this book provides a foundation for thinking about the certification and risk management of machine learning systems, and allows them to use their domain expertise to build better machine learning systems.

Experienced Artist Skilled practitioners of machine learning can plug and play different tools and libraries into an analysis pipeline. The stereotypical practitioner would be a data scientist or engineer who understands machine learning interfaces and their use cases, and is able to perform wonderful feats of prediction from data. This is similar to a virtuoso playing music, where highly skilled practitioners can bring existing instruments to life and bring enjoyment to their audience. Using the mathematics presented here as a primer, practitioners would be able to understand the benefits and limits of their favorite method, and to extend and generalize existing machine learning algorithms. We hope that this book provides the impetus for more rigorous and principled development of machine learning methods.

Fledgling Composer As machine learning is applied to new domains, developers of machine learning need to develop new methods and extend existing algorithms. They are often researchers who need to understand the mathematical basis of machine learning and uncover relationships between different tasks. This is similar to composers of music who, within the rules and structure of musical theory, create new and amazing pieces. We hope this book provides a high-level overview of other technical books for people who want to become composers of machine learning. There is a great need in society for new researchers who are able to propose and explore novel approaches for attacking the many challenges of learning from data.

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Table of Symbols

Symbol	Typical meaning
$a, b, c, \alpha, \beta, \gamma$	Scalars are lowercase
$oldsymbol{x},oldsymbol{y},oldsymbol{z},$	Vectors are bold lowercase
A,B,C	Matrices are bold uppercase
$oldsymbol{x}^ op, oldsymbol{A}^ op$	Transpose of a vector or matrix
$oldsymbol{A}^{-1}$	Inverse of a matrix
$\langle oldsymbol{x}, oldsymbol{y} angle$	
$egin{array}{c} \langle oldsymbol{x}, oldsymbol{y} angle \ oldsymbol{x}^ op oldsymbol{y} \end{array}$	Inner product of x and y
•	Dot product of x and y
$B = (\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3)$	(Ordered) tuple Matrix of column vectors stacked horizontally
$B = [b_1, b_2, b_3]$	•
$\mathcal{B} = \{oldsymbol{b}_1, oldsymbol{b}_2, oldsymbol{b}_3\}$	Set of vectors (unordered)
\mathbb{Z}, \mathbb{N}	Integers and natural numbers, respectively
\mathbb{R}, \mathbb{C}	Real and complex numbers, respectively
\mathbb{R}^n	n-dimensional vector space of real numbers
$\forall x$	Universal quantifier: for all x
$\exists x$	Existential quantifier: there exists x
a := b	a is defined as b b is defined as a
a =: b	
$a \propto b$	a is proportional to b, i.e., $a = \text{constant} \cdot b$
$g \circ f$	Function composition: " g after f "
\Leftrightarrow \Rightarrow	If and only if
	Implies
\mathcal{A},\mathcal{C}	Sets
$a \in \mathcal{A}$	a is an element of set \mathcal{A}
	Empty set A without B : the set of elements in A but not in B
$egin{array}{c} \mathcal{A} ackslash \mathcal{B} \ D \end{array}$	Number of dimensions; indexed by $d = 1,, D$
$\stackrel{D}{N}$	Number of data points; indexed by $n = 1,, N$
$oldsymbol{I_m}$	Identity matrix of size $m \times m$
	Matrix of size $m \times m$
$0_{m,n}$	Matrix of ones of size $m \times n$
$1_{m,n}$	Standard/canonical vector (where i is the component that is 1)
$oldsymbol{e}_i \ ext{dim}$	Dimensionality of vector space
$\operatorname{rk}(oldsymbol{A})$	Rank of matrix A
$\operatorname{Im}(\Phi)$	Image of linear mapping Φ
$\ker(\Phi)$	Kernel (null space) of a linear mapping Φ
$\operatorname{span}[\boldsymbol{b}_1]$	Span (generating set) of b_1
$\operatorname{tr}(\boldsymbol{A})$	Trace of A
$\det(\boldsymbol{A})$	Determinant of A
•	Absolute value or determinant (depending on context)
•	Norm; Euclidean, unless specified
$\stackrel{\scriptscriptstyle{ }}{\lambda}$	Eigenvalue or Lagrange multiplier
$\stackrel{\scriptstyle \wedge}{E_{\lambda}}$	Eigenspace corresponding to eigenvalue λ
L_{λ}	Lifetispace corresponding to eigenvalue /

Symbol	Typical meaning
$\overline{x \perp y}$	Vectors x and y are orthogonal
V	Vector space
V^{\perp}	Orthogonal complement of vector space V
$\sum_{n=1}^{N} x_n$ $\prod_{n=1}^{N} x_n$	Sum of the x_n : $x_1 + \ldots + x_N$
$\prod_{n=1}^{N} x_n$	Product of the x_n : $x_1 \cdot \ldots \cdot x_N$
$oldsymbol{ heta}$	Parameter vector
$egin{array}{c} oldsymbol{ heta} & rac{\partial f}{\partial x} \ rac{\partial f}{\nabla} & \end{array}$	Partial derivative of f with respect to x
$\frac{\mathrm{d}f}{\mathrm{d}x}$	Total derivative of f with respect to x
$\overset{\mathrm{d}x}{ abla}$	Gradient
$f_* = \min_x f(x)$	The smallest function value of f
$x_* \in \arg\min_x f(x)$	The value x_* that minimizes f (note: $arg min returns a set of values)$
$\mathfrak L$	Lagrangian
${\cal L}$	Negative log-likelihood
$\binom{n}{k}$	Binomial coefficient, n choose k
$\mathbb{V}_X[oldsymbol{x}]$	Variance of x with respect to the random variable X
$\mathbb{E}_X[oldsymbol{x}]$	Expectation of x with respect to the random variable X
$\mathrm{Cov}_{X,Y}[oldsymbol{x},oldsymbol{y}]$	Covariance between x and y .
$X \perp\!\!\!\perp Y \mid Z$	X is conditionally independent of Y given Z
$X \sim p$	Random variable X is distributed according to p
$\mathcal{N}(oldsymbol{\mu},oldsymbol{\Sigma})$	Gaussian distribution with mean μ and covariance Σ
$\operatorname{Ber}(\mu)$	Bernoulli distribution with parameter μ
$\operatorname{Bin}(N,\mu)$	Binomial distribution with parameters N, μ
$Beta(\alpha,\beta)$	Beta distribution with parameters α, β

Table of Abbreviations and Acronyms

Acronym	Meaning
e.g.	Exempli gratia (Latin: for example)
GMM	Gaussian mixture model
i.e.	Id est (Latin: this means)
i.i.d.	Independent, identically distributed
MAP	Maximum a posteriori
MLE	Maximum likelihood estimation/estimator
ONB	Orthonormal basis
PCA	Principal component analysis
PPCA	Probabilistic principal component analysis
REF	Row-echelon form
SPD	Symmetric, positive definite
SVM	Support vector machine

Part I

Mathematical Foundations

Introduction and Motivation

Machine learning is about designing algorithms that automatically extract valuable information from data. The emphasis here is on "automatic", i.e., machine learning is concerned about general-purpose methodologies that can be applied to many datasets, while producing something that is meaningful. There are three concepts that are at the core of machine learning: data, a model, and learning.

Since machine learning is inherently data driven, data is at the core of machine learning. The goal of machine learning is to design generalpurpose methodologies to extract valuable patterns from data, ideally without much domain-specific expertise. For example, given a large corpus of documents (e.g., books in many libraries), machine learning methods can be used to automatically find relevant topics that are shared across documents (Hoffman et al., 2010). To achieve this goal, we design models that are typically related to the process that generates data, similar to the dataset we are given. For example, in a regression setting, the model would describe a function that maps inputs to real-valued outputs. To paraphrase Mitchell (1997): A model is said to learn from data if its performance on a given task improves after the data is taken into account. The goal is to find good models that generalize well to yet unseen data, which we may care about in the future. Learning can be understood as a way to automatically find patterns and structure in data by optimizing the parameters of the model.

....

model

learning

While machine learning has seen many success stories, and software is readily available to design and train rich and flexible machine learning systems, we believe that the mathematical foundations of machine learning are important in order to understand fundamental principles upon which more complicated machine learning systems are built. Understanding these principles can facilitate creating new machine learning solutions, understanding and debugging existing approaches, and learning about the inherent assumptions and limitations of the methodologies we are working with.

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1.1 Finding Words for Intuitions

A challenge we face regularly in machine learning is that concepts and words are slippery, and a particular component of the machine learning system can be abstracted to different mathematical concepts. For example, the word "algorithm" is used in at least two different senses in the context of machine learning. In the first sense, we use the phrase "machine learning algorithm" to mean a system that makes predictions based on input data. We refer to these algorithms as *predictors*. In the second sense, we use the exact same phrase "machine learning algorithm" to mean a system that adapts some internal parameters of the predictor so that it performs well on future unseen input data. Here we refer to this adaptation as *training* a system.

This book will not resolve the issue of ambiguity, but we want to highlight upfront that, depending on the context, the same expressions can mean different things. However, we attempt to make the context sufficiently clear to reduce the level of ambiguity.

The first part of this book introduces the mathematical concepts and foundations needed to talk about the three main components of a machine learning system: data, models, and learning. We will briefly outline these components here, and we will revisit them again in Chapter 8 once we have discussed the necessary mathematical concepts.

While not all data is numerical, it is often useful to consider data in a number format. In this book, we assume that *data* has already been appropriately converted into a numerical representation suitable for reading into a computer program. Therefore, we think of data as vectors. As another illustration of how subtle words are, there are (at least) three different ways to think about vectors: a vector as an array of numbers (a computer science view), a vector as an arrow with a direction and magnitude (a physics view), and a vector as an object that obeys addition and scaling (a mathematical view).

A *model* is typically used to describe a process for generating data, similar to the dataset at hand. Therefore, good models can also be thought of as simplified versions of the real (unknown) data-generating process, capturing aspects that are relevant for modeling the data and extracting hidden patterns from it. A good model can then be used to predict what would happen in the real world without performing real-world experiments.

We now come to the crux of the matter, the *learning* component of machine learning. Assume we are given a dataset and a suitable model. *Training* the model means to use the data available to optimize some parameters of the model with respect to a utility function that evaluates how well the model predicts the training data. Most training methods can be thought of as an approach analogous to climbing a hill to reach its peak. In this analogy, the peak of the hill corresponds to a maximum of some

predictor

training

data as vectors

model

learning

desired performance measure. However, in practice, we are interested in the model to perform well on unseen data. Performing well on data that we have already seen (training data) may only mean that we found a good way to memorize the data. However, this may not generalize well to unseen data, and, in practical applications, we often need to expose our machine learning system to situations that it has not encountered before.

Let us summarize the main concepts of machine learning that we cover in this book:

- We represent data as vectors.
- We choose an appropriate model, either using the probabilistic or optimization view.
- We learn from available data by using numerical optimization methods with the aim that the model performs well on data not used for training.

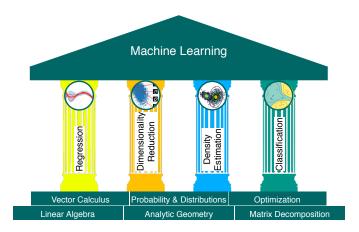
1.2 Two Ways to Read This Book

We can consider two strategies for understanding the mathematics for machine learning:

- **Bottom-up:** Building up the concepts from foundational to more advanced. This is often the preferred approach in more technical fields, such as mathematics. This strategy has the advantage that the reader at all times is able to rely on their previously learned concepts. Unfortunately, for a practitioner many of the foundational concepts are not particularly interesting by themselves, and the lack of motivation means that most foundational definitions are quickly forgotten.
- **Top-down:** Drilling down from practical needs to more basic requirements. This goal-driven approach has the advantage that the readers know at all times why they need to work on a particular concept, and there is a clear path of required knowledge. The downside of this strategy is that the knowledge is built on potentially shaky foundations, and the readers have to remember a set of words that they do not have any way of understanding.

We decided to write this book in a modular way to separate foundational (mathematical) concepts from applications so that this book can be read in both ways. The book is split into two parts, where Part I lays the mathematical foundations and Part II applies the concepts from Part I to a set of fundamental machine learning problems, which form four pillars of machine learning as illustrated in Figure 1.1: regression, dimensionality reduction, density estimation, and classification. Chapters in Part I mostly build upon the previous ones, but it is possible to skip a chapter and work backward if necessary. Chapters in Part II are only loosely coupled and can be read in any order. There are many pointers forward and backward

Figure 1.1 The foundations and four pillars of machine learning.



between the two parts of the book to link mathematical concepts with machine learning algorithms.

Of course there are more than two ways to read this book. Most readers learn using a combination of top-down and bottom-up approaches, sometimes building up basic mathematical skills before attempting more complex concepts, but also choosing topics based on applications of machine learning.

Part I Is about Mathematics

The four pillars of machine learning we cover in this book (see Figure 1.1) require a solid mathematical foundation, which is laid out in Part I.

We represent numerical data as vectors and represent a table of such data as a matrix. The study of vectors and matrices is called *linear algebra*, which we introduce in Chapter 2. The collection of vectors as a matrix is also described there.

Given two vectors representing two objects in the real world, we want to make statements about their similarity. The idea is that vectors that are similar should be predicted to have similar outputs by our machine learning algorithm (our predictor). To formalize the idea of similarity between vectors, we need to introduce operations that take two vectors as input and return a numerical value representing their similarity. The construction of similarity and distances is central to *analytic geometry* and is discussed in Chapter 3.

In Chapter 4, we introduce some fundamental concepts about matrices and *matrix decomposition*. Some operations on matrices are extremely useful in machine learning, and they allow for an intuitive interpretation of the data and more efficient learning.

We often consider data to be noisy observations of some true underlying signal. We hope that by applying machine learning we can identify the signal from the noise. This requires us to have a language for quantifying what "noise" means. We often would also like to have predictors that

linear algebra

analytic geometry

matrix decomposition

15

allow us to express some sort of uncertainty, e.g., to quantify the confidence we have about the value of the prediction at a particular test data point. Quantification of uncertainty is the realm of *probability theory* and is covered in Chapter 6.

probability theory

To train machine learning models, we typically find parameters that maximize some performance measure. Many optimization techniques require the concept of a gradient, which tells us the direction in which to search for a solution. Chapter 5 is about *vector calculus* and details the concept of gradients, which we subsequently use in Chapter 7, where we talk about *optimization* to find maxima/minima of functions.

vector calculus

optimization

Part II Is about Machine Learning

The second part of the book introduces *four pillars of machine learning* as shown in Figure 1.1. We illustrate how the mathematical concepts introduced in the first part of the book are the foundation for each pillar. Broadly speaking, chapters are ordered by difficulty (in ascending order).

In Chapter 8, we restate the three components of machine learning (data, models, and parameter estimation) in a mathematical fashion. In addition, we provide some guidelines for building experimental set-ups that guard against overly optimistic evaluations of machine learning systems. Recall that the goal is to build a predictor that performs well on unseen data.

In Chapter 9, we will have a close look at *linear regression*, where our objective is to find functions that map inputs $x \in \mathbb{R}^D$ to corresponding observed function values $y \in \mathbb{R}$, which we can interpret as the labels of their respective inputs. We will discuss classical model fitting (parameter estimation) via maximum likelihood and maximum a posteriori estimation, as well as Bayesian linear regression, where we integrate the parameters out instead of optimizing them.

linear regression

Chapter 10 focuses on *dimensionality reduction*, the second pillar in Figure 1.1, using principal component analysis. The key objective of dimensionality reduction is to find a compact, lower-dimensional representation of high-dimensional data $\boldsymbol{x} \in \mathbb{R}^D$, which is often easier to analyze than the original data. Unlike regression, dimensionality reduction is only concerned about modeling the data – there are no labels associated with a data point \boldsymbol{x} .

dimensionality reduction

In Chapter 11, we will move to our third pillar: density estimation. The objective of density estimation is to find a probability distribution that describes a given dataset. We will focus on Gaussian mixture models for this purpose, and we will discuss an iterative scheme to find the parameters of this model. As in dimensionality reduction, there are no labels associated with the data points $\boldsymbol{x} \in \mathbb{R}^D$. However, we do not seek a low-dimensional representation of the data. Instead, we are interested in a density model that describes the data.

density estimation

Chapter 12 concludes the book with an in-depth discussion of the fourth

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classification

pillar: classification. We will discuss classification in the context of support vector machines. Similar to regression (Chapter 9), we have inputs \boldsymbol{x} and corresponding labels \boldsymbol{y} . However, unlike regression, where the labels were real-valued, the labels in classification are integers, which requires special care.

1.3 Exercises and Feedback

We provide some exercises in Part I, which can be done mostly by pen and paper. For Part II, we provide programming tutorials (jupyter notebooks) to explore some properties of the machine learning algorithms we discuss in this book.

We appreciate that Cambridge University Press strongly supports our aim to democratize education and learning by making this book freely available for download at

https://mml-book.com

where tutorials, errata, and additional materials can be found. Mistakes can be reported and feedback provided using the preceding URL.

Linear Algebra

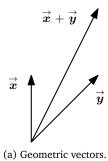


When formalizing intuitive concepts, a common approach is to construct a set of objects (symbols) and a set of rules to manipulate these objects. This is known as an *algebra*. Linear algebra is the study of vectors and certain rules to manipulate vectors. The vectors many of us know from school are called "geometric vectors", which are usually denoted by a small arrow above the letter, e.g., \overrightarrow{x} and \overrightarrow{y} . In this book, we discuss more general concepts of vectors and use a bold letter to represent them, e.g., x and y.

algebra

In general, vectors are special objects that can be added together and multiplied by scalars to produce another object of the same kind. From an abstract mathematical viewpoint, any object that satisfies these two properties can be considered a vector. Here are some examples of such vector objects:

- 1. Geometric vectors. This example of a vector may be familiar from high school mathematics and physics. Geometric vectors see Figure 2.1(a) are directed segments, which can be drawn (at least in two dimensions). Two geometric vectors \overrightarrow{x} , \overrightarrow{y} can be added, such that $\overrightarrow{x}+\overrightarrow{y}=\overrightarrow{z}$ is another geometric vector. Furthermore, multiplication by a scalar $\lambda \overrightarrow{x}$, $\lambda \in \mathbb{R}$, is also a geometric vector. In fact, it is the original vector scaled by λ . Therefore, geometric vectors are instances of the vector concepts introduced previously. Interpreting vectors as geometric vectors enables us to use our intuitions about direction and magnitude to reason about mathematical operations.
- 2. Polynomials are also vectors; see Figure 2.1(b): Two polynomials can



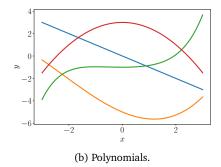


Figure 2.1
Different types of vectors. Vectors can be surprising objects, including (a) geometric vectors and (b) polynomials.

be added together, which results in another polynomial; and they can be multiplied by a scalar $\lambda \in \mathbb{R}$, and the result is a polynomial as well. Therefore, polynomials are (rather unusual) instances of vectors. Note that polynomials are very different from geometric vectors. While geometric vectors are concrete "drawings", polynomials are abstract concepts. However, they are both vectors in the sense previously described.

- 3. Audio signals are vectors. Audio signals are represented as a series of numbers. We can add audio signals together, and their sum is a new audio signal. If we scale an audio signal, we also obtain an audio signal. Therefore, audio signals are a type of vector, too.
- 4. Elements of \mathbb{R}^n (tuples of n real numbers) are vectors. \mathbb{R}^n is more abstract than polynomials, and it is the concept we focus on in this book. For instance,

$$\boldsymbol{a} = \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \in \mathbb{R}^3 \tag{2.1}$$

is an example of a triplet of numbers. Adding two vectors $a, b \in \mathbb{R}^n$ component-wise results in another vector: $a + b = c \in \mathbb{R}^n$. Moreover, multiplying $a \in \mathbb{R}^n$ by $\lambda \in \mathbb{R}$ results in a scaled vector $\lambda a \in \mathbb{R}^n$. Considering vectors as elements of \mathbb{R}^n has an additional benefit that it loosely corresponds to arrays of real numbers on a computer. Many programming languages support array operations, which allow for convenient implementation of algorithms that involve vector operations.

Linear algebra focuses on the similarities between these vector concepts. We can add them together and multiply them by scalars. We will largely focus on vectors in \mathbb{R}^n since most algorithms in linear algebra are formulated in \mathbb{R}^n . We will see in Chapter 8 that we often consider data to be represented as vectors in \mathbb{R}^n . In this book, we will focus on finite-dimensional vector spaces, in which case there is a 1:1 correspondence between any kind of vector and \mathbb{R}^n . When it is convenient, we will use intuitions about geometric vectors and consider array-based algorithms.

One major idea in mathematics is the idea of "closure". This is the question: What is the set of all things that can result from my proposed operations? In the case of vectors: What is the set of vectors that can result by starting with a small set of vectors, and adding them to each other and scaling them? This results in a vector space (Section 2.4). The concept of a vector space and its properties underlie much of machine learning. The concepts introduced in this chapter are summarized in Figure 2.2.

This chapter is mostly based on the lecture notes and books by Drumm and Weil (2001), Strang (2003), Hogben (2013), Liesen and Mehrmann (2015), as well as Pavel Grinfeld's Linear Algebra series. Other excellent

Be careful to check whether array operations actually perform vector operations when implementing on a computer.

Pavel Grinfeld's series on linear algebra: http://tinyurl.com/nahclwm Gilbert Strang's course on linear algebra: http://tinyurl.com/29p5q8j 3Blue1Brown series on linear algebra: https://tinyurl.com/h5g4kps

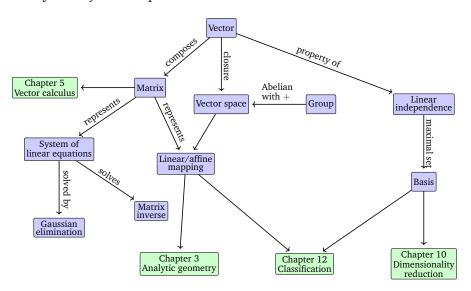


Figure 2.2 A mind map of the concepts introduced in this chapter, along with where they are used in other parts of the book.

resources are Gilbert Strang's Linear Algebra course at MIT and the Linear Algebra Series by 3Blue1Brown.

Linear algebra plays an important role in machine learning and general mathematics. The concepts introduced in this chapter are further expanded to include the idea of geometry in Chapter 3. In Chapter 5, we will discuss vector calculus, where a principled knowledge of matrix operations is essential. In Chapter 10, we will use projections (to be introduced in Section 3.8) for dimensionality reduction with principal component analysis (PCA). In Chapter 9, we will discuss linear regression, where linear algebra plays a central role for solving least-squares problems.

2.1 Systems of Linear Equations

Systems of linear equations play a central part of linear algebra. Many problems can be formulated as systems of linear equations, and linear algebra gives us the tools for solving them.

Example 2.1

A company produces products N_1, \ldots, N_n for which resources R_1, \ldots, R_m are required. To produce a unit of product N_j , a_{ij} units of resource R_i are needed, where $i=1,\ldots,m$ and $j=1,\ldots,n$.

The objective is to find an optimal production plan, i.e., a plan of how many units x_j of product N_j should be produced if a total of b_i units of resource R_i are available and (ideally) no resources are left over.

If we produce x_1, \ldots, x_n units of the corresponding products, we need

a total of

$$a_{i1}x_1 + \dots + a_{in}x_n \tag{2.2}$$

many units of resource R_i . An optimal production plan $(x_1, \ldots, x_n) \in \mathbb{R}^n$, therefore, has to satisfy the following system of equations:

$$a_{11}x_1 + \dots + a_{1n}x_n = b_1$$

 \vdots , (2.3)
 $a_{m1}x_1 + \dots + a_{mn}x_n = b_m$

where $a_{ij} \in \mathbb{R}$ and $b_i \in \mathbb{R}$.

system of linear equations solution Equation (2.3) is the general form of a system of linear equations, and x_1, \ldots, x_n are the unknowns of this system. Every n-tuple $(x_1, \ldots, x_n) \in \mathbb{R}^n$ that satisfies (2.3) is a solution of the linear equation system.

Example 2.2

The system of linear equations

has *no solution*: Adding the first two equations yields $2x_1+3x_3=5$, which contradicts the third equation (3).

Let us have a look at the system of linear equations

From the first and third equation, it follows that $x_1 = 1$. From (1)+(2), we get $2x_1 + 3x_3 = 5$, i.e., $x_3 = 1$. From (3), we then get that $x_2 = 1$. Therefore, (1,1,1) is the only possible and *unique solution* (verify that (1,1,1) is a solution by plugging in).

As a third example, we consider

Since (1)+(2)=(3), we can omit the third equation (redundancy). From (1) and (2), we get $2x_1=5-3x_3$ and $2x_2=1+x_3$. We define $x_3=a\in\mathbb{R}$ as a free variable, such that any triplet

$$\left(\frac{5}{2} - \frac{3}{2}a, \frac{1}{2} + \frac{1}{2}a, a\right), \quad a \in \mathbb{R}$$
 (2.7)



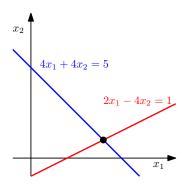


Figure 2.3 The solution space of a system of two linear equations with two variables can be geometrically interpreted as the intersection of two lines. Every linear equation represents a line.

is a solution of the system of linear equations, i.e., we obtain a solution set that contains *infinitely many* solutions.

In general, for a real-valued system of linear equations we obtain either no, exactly one, or infinitely many solutions. Linear regression (Chapter 9) solves a version of Example 2.1 when we cannot solve the system of linear equations.

Remark (Geometric Interpretation of Systems of Linear Equations). In a system of linear equations with two variables x_1, x_2 , each linear equation defines a line on the x_1x_2 -plane. Since a solution to a system of linear equations must satisfy all equations simultaneously, the solution set is the intersection of these lines. This intersection set can be a line (if the linear equations describe the same line), a point, or empty (when the lines are parallel). An illustration is given in Figure 2.3 for the system

$$4x_1 + 4x_2 = 5$$

$$2x_1 - 4x_2 = 1$$
(2.8)

where the solution space is the point $(x_1, x_2) = (1, \frac{1}{4})$. Similarly, for three variables, each linear equation determines a plane in three-dimensional space. When we intersect these planes, i.e., satisfy all linear equations at the same time, we can obtain a solution set that is a plane, a line, a point or empty (when the planes have no common intersection).

For a systematic approach to solving systems of linear equations, we will introduce a useful compact notation. We collect the coefficients a_{ij} into vectors and collect the vectors into matrices. In other words, we write the system from (2.3) in the following form:

$$\begin{bmatrix} a_{11} \\ \vdots \\ a_{m1} \end{bmatrix} x_1 + \begin{bmatrix} a_{12} \\ \vdots \\ a_{m2} \end{bmatrix} x_2 + \dots + \begin{bmatrix} a_{1n} \\ \vdots \\ a_{mn} \end{bmatrix} x_n = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}$$
 (2.9)

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$$\iff \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & & \vdots \\ a_{m1} & \cdots & a_{mn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \vdots \\ b_m \end{bmatrix}. \tag{2.10}$$

In the following, we will have a close look at these *matrices* and define computation rules. We will return to solving linear equations in Section 2.3.

2.2 Matrices

Matrices play a central role in linear algebra. They can be used to compactly represent systems of linear equations, but they also represent linear functions (linear mappings) as we will see later in Section 2.7. Before we discuss some of these interesting topics, let us first define what a matrix is and what kind of operations we can do with matrices. We will see more properties of matrices in Chapter 4.

Definition 2.1 (Matrix). With $m, n \in \mathbb{N}$ a real-valued (m, n) matrix A is an $m \cdot n$ -tuple of elements a_{ij} , $i = 1, \ldots, m, j = 1, \ldots, n$, which is ordered according to a rectangular scheme consisting of m rows and n columns:

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1n} \\ a_{21} & a_{22} & \cdots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{m1} & a_{m2} & \cdots & a_{mn} \end{bmatrix}, \quad a_{ij} \in \mathbb{R}.$$
 (2.11)

By convention (1, n)-matrices are called *rows* and (m, 1)-matrices are called *columns*. These special matrices are also called *row/column vectors*.

 $\mathbb{R}^{m \times n}$ is the set of all real-valued (m,n)-matrices. $\boldsymbol{A} \in \mathbb{R}^{m \times n}$ can be equivalently represented as $\boldsymbol{a} \in \mathbb{R}^{mn}$ by stacking all n columns of the matrix into a long vector; see Figure 2.4.

2.2.1 Matrix Addition and Multiplication

The sum of two matrices $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{m \times n}$ is defined as the elementwise sum, i.e.,

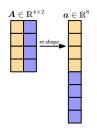
$$\mathbf{A} + \mathbf{B} := \begin{bmatrix} a_{11} + b_{11} & \cdots & a_{1n} + b_{1n} \\ \vdots & & \vdots \\ a_{m1} + b_{m1} & \cdots & a_{mn} + b_{mn} \end{bmatrix} \in \mathbb{R}^{m \times n}.$$
 (2.12)

For matrices $A \in \mathbb{R}^{m \times n}$, $B \in \mathbb{R}^{n \times k}$, the elements c_{ij} of the product $C = AB \in \mathbb{R}^{m \times k}$ are computed as

$$c_{ij} = \sum_{l=1}^{n} a_{il} b_{lj}, \qquad i = 1, \dots, m, \quad j = 1, \dots, k.$$
 (2.13)

matrix

row
column
row vector
column vector
Figure 2.4 By
stacking its
columns, a matrix A
can be represented
as a long vector a.



Note the size of the matrices.

C = np.einsum('il, lj', A, B)

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This means, to compute element c_{ij} we multiply the elements of the ith row of A with the jth column of B and sum them up. Later in Section 3.2, we will call this the dot product of the corresponding row and column. In cases, where we need to be explicit that we are performing multiplication, we use the notation $A \cdot B$ to denote multiplication (explicitly showing "·").

Remark. Matrices can only be multiplied if their "neighboring" dimensions match. For instance, an $n \times k$ -matrix \boldsymbol{A} can be multiplied with a $k \times m$ -matrix \boldsymbol{B} , but only from the left side:

$$\underbrace{A}_{n \times k} \underbrace{B}_{k \times m} = \underbrace{C}_{n \times m} \tag{2.14}$$

The product BA is not defined if $m \neq n$ since the neighboring dimensions do not match. \diamondsuit

Remark. Matrix multiplication is *not* defined as an element-wise operation on matrix elements, i.e., $c_{ij} \neq a_{ij}b_{ij}$ (even if the size of $\boldsymbol{A}, \boldsymbol{B}$ was chosen appropriately). This kind of element-wise multiplication often appears in programming languages when we multiply (multi-dimensional) arrays with each other, and is called a *Hadamard product*. \diamondsuit

in \boldsymbol{A} and \boldsymbol{n} rows in \boldsymbol{B} so that we can compute $a_{il}b_{lj}$ for $l=1,\ldots,n$. Commonly, the dot product between two vectors $\boldsymbol{a},\boldsymbol{b}$ is denoted by $\boldsymbol{a}^{\top}\boldsymbol{b}$ or $\langle \boldsymbol{a},\boldsymbol{b} \rangle$.

There are n columns

Hadamard product

Example 2.3

For
$$\boldsymbol{A} = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{bmatrix} \in \mathbb{R}^{2 \times 3}$$
, $\boldsymbol{B} = \begin{bmatrix} 0 & 2 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \in \mathbb{R}^{3 \times 2}$, we obtain

$$\mathbf{AB} = \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{bmatrix} \begin{bmatrix} 0 & 2 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 2 & 3 \\ 2 & 5 \end{bmatrix} \in \mathbb{R}^{2 \times 2}, \tag{2.15}$$

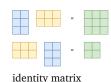
$$\boldsymbol{B}\boldsymbol{A} = \begin{bmatrix} 0 & 2 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 4 & 2 \\ -2 & 0 & 2 \\ 3 & 2 & 1 \end{bmatrix} \in \mathbb{R}^{3 \times 3}.$$
 (2.16)

From this example, we can already see that matrix multiplication is not commutative, i.e., $AB \neq BA$; see also Figure 2.5 for an illustration.

Definition 2.2 (Identity Matrix). In $\mathbb{R}^{n \times n}$, we define the *identity matrix*

$$I_{n} := \begin{bmatrix} 1 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & 0 & \cdots & 1 \end{bmatrix} \in \mathbb{R}^{n \times n}$$
(2.17)

Figure 2.5 Even if both matrix multiplications AB and BA are defined, the dimensions of the results can be different.



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as the $n \times n$ -matrix containing 1 on the diagonal and 0 everywhere else.

Now that we defined matrix multiplication, matrix addition and the identity matrix, let us have a look at some properties of matrices:

associativity:

**Associativity:

$$\forall A \in \mathbb{R}^{m \times n}, B \in \mathbb{R}^{n \times p}, C \in \mathbb{R}^{p \times q} : (AB)C = A(BC)$$
 (2.18)

distributivity

■ *Distributivity*:

$$orall A, B \in \mathbb{R}^{m imes n}, C, D \in \mathbb{R}^{n imes p} : (A+B)C = AC+BC$$
 (2.19a)
 $A(C+D) = AC+AD$ (2.19b)

• Multiplication with the identity matrix:

$$\forall A \in \mathbb{R}^{m \times n} : I_m A = A I_n = A \tag{2.20}$$

Note that $I_m \neq I_n$ for $m \neq n$.

2.2.2 Inverse and Transpose

Definition 2.3 (Inverse). Consider a square matrix $A \in \mathbb{R}^{n \times n}$. Let matrix $B \in \mathbb{R}^{n \times n}$ have the property that $AB = I_n = BA$. B is called the *inverse* of A and denoted by A^{-1} .

Unfortunately, not every matrix A possesses an inverse A^{-1} . If this inverse does exist, A is called regular/invertible/nonsingular, otherwise singular/noninvertible. When the matrix inverse exists, it is unique. In Section 2.3, we will discuss a general way to compute the inverse of a matrix by solving a system of linear equations.

Remark (Existence of the Inverse of a 2×2 -matrix). Consider a matrix

$$A := \begin{bmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{bmatrix} \in \mathbb{R}^{2 \times 2}$$
 (2.21)

If we multiply A with

$$\mathbf{A}' := \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix} \tag{2.22}$$

we obtain

$$\mathbf{A}\mathbf{A}' = \begin{bmatrix} a_{11}a_{22} - a_{12}a_{21} & 0\\ 0 & a_{11}a_{22} - a_{12}a_{21} \end{bmatrix} = (a_{11}a_{22} - a_{12}a_{21})\mathbf{I}.$$
(2.23)

Therefore,

$$\boldsymbol{A}^{-1} = \frac{1}{a_{11}a_{22} - a_{12}a_{21}} \begin{bmatrix} a_{22} & -a_{12} \\ -a_{21} & a_{11} \end{bmatrix}$$
 (2.24)

if and only if $a_{11}a_{22} - a_{12}a_{21} \neq 0$. In Section 4.1, we will see that $a_{11}a_{22} - a_{12}a_{21} \neq 0$.

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A square matrix possesses the same number of columns and rows. inverse

regular invertible nonsingular singular noninvertible

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 $a_{12}a_{21}$ is the determinant of a 2×2 -matrix. Furthermore, we can generally use the determinant to check whether a matrix is invertible. \diamondsuit

Example 2.4 (Inverse Matrix)

The matrices

$$\mathbf{A} = \begin{bmatrix} 1 & 2 & 1 \\ 4 & 4 & 5 \\ 6 & 7 & 7 \end{bmatrix}, \quad \mathbf{B} = \begin{bmatrix} -7 & -7 & 6 \\ 2 & 1 & -1 \\ 4 & 5 & -4 \end{bmatrix}$$
 (2.25)

are inverse to each other since AB = I = BA.

Definition 2.4 (Transpose). For $A \in \mathbb{R}^{m \times n}$ the matrix $B \in \mathbb{R}^{n \times m}$ with $b_{ij} = a_{ji}$ is called the *transpose* of A. We write $B = A^{\top}$.

In general, A^{\top} can be obtained by writing the columns of A as the rows of A^{\top} . The following are important properties of inverses and transposes:

$$AA^{-1} = I = A^{-1}A (2.26)$$

$$(AB)^{-1} = B^{-1}A^{-1} (2.27)$$

$$(A+B)^{-1} \neq A^{-1} + B^{-1}$$
 (2.28)

$$(\boldsymbol{A}^{\top})^{\top} = \boldsymbol{A} \tag{2.29}$$

$$(\boldsymbol{A} + \boldsymbol{B})^{\top} = \boldsymbol{A}^{\top} + \boldsymbol{B}^{\top} \tag{2.30}$$

$$(\mathbf{A}\mathbf{B})^{\top} = \mathbf{B}^{\top}\mathbf{A}^{\top} \tag{2.31}$$

Definition 2.5 (Symmetric Matrix). A matrix $A \in \mathbb{R}^{n \times n}$ is *symmetric* if symmetric matrix $A = A^{\top}$.

square matrix

transpose

The main diagonal

(sometimes called

"principal diagonal", "primary diagonal", "leading diagonal",

or "major diagonal") of a matrix A is the

collection of entries

 A_{ij} where i = j.

The scalar case of

 $\frac{1}{2+4} = \frac{1}{6} \neq \frac{1}{2} + \frac{1}{4}$.

(2.28) is

Note that only (n,n)-matrices can be symmetric. Generally, we call (n,n)-matrices also *square matrices* because they possess the same number of rows and columns. Moreover, if \boldsymbol{A} is invertible, then so is \boldsymbol{A}^{\top} , and $(\boldsymbol{A}^{-1})^{\top} = (\boldsymbol{A}^{\top})^{-1} =: \boldsymbol{A}^{-\top}$.

Remark (Sum and Product of Symmetric Matrices). The sum of symmetric matrices $A, B \in \mathbb{R}^{n \times n}$ is always symmetric. However, although their product is always defined, it is generally not symmetric:

$$\begin{bmatrix} 1 & 0 \\ 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 1 & 1 \end{bmatrix} = \begin{bmatrix} 1 & 1 \\ 0 & 0 \end{bmatrix}. \tag{2.32}$$



2.2.3 Multiplication by a Scalar

Let us look at what happens to matrices when they are multiplied by a scalar $\lambda \in \mathbb{R}$. Let $A \in \mathbb{R}^{m \times n}$ and $\lambda \in \mathbb{R}$. Then $\lambda A = K$, $K_{ij} = \lambda a_{ij}$. Practically, λ scales each element of A. For $\lambda, \psi \in \mathbb{R}$, the following holds:

associativity

distributivity

• Associativity: $(\lambda \psi) C = \lambda(\psi C), \quad C \in \mathbb{R}^{m \times n}$

■ $\lambda(BC) = (\lambda B)C = B(\lambda C) = (BC)\lambda$, $B \in \mathbb{R}^{m \times n}, C \in \mathbb{R}^{n \times k}$. Note that this allows us to move scalar values around.

• $(\lambda C)^{\top} = C^{\top} \lambda^{\top} = C^{\top} \lambda = \lambda C^{\top}$ since $\lambda = \lambda^{\top}$ for all $\lambda \in \mathbb{R}$.

Distributivity:

$$(\lambda + \psi)C = \lambda C + \psi C, \quad C \in \mathbb{R}^{m \times n}$$

 $\lambda(B + C) = \lambda B + \lambda C, \quad B, C \in \mathbb{R}^{m \times n}$

Example 2.5 (Distributivity)

If we define

$$C := \begin{bmatrix} 1 & 2 \\ 3 & 4 \end{bmatrix}, \tag{2.33}$$

then for any $\lambda, \psi \in \mathbb{R}$ we obtain

$$(\lambda + \psi)\mathbf{C} = \begin{bmatrix} (\lambda + \psi)1 & (\lambda + \psi)2\\ (\lambda + \psi)3 & (\lambda + \psi)4 \end{bmatrix} = \begin{bmatrix} \lambda + \psi & 2\lambda + 2\psi\\ 3\lambda + 3\psi & 4\lambda + 4\psi \end{bmatrix}$$
(2.34a)
$$= \begin{bmatrix} \lambda & 2\lambda\\ 3\lambda & 4\lambda \end{bmatrix} + \begin{bmatrix} \psi & 2\psi\\ 3\psi & 4\psi \end{bmatrix} = \lambda\mathbf{C} + \psi\mathbf{C}.$$
(2.34b)

2.2.4 Compact Representations of Systems of Linear Equations

If we consider the system of linear equations

$$2x_1 + 3x_2 + 5x_3 = 1$$

 $4x_1 - 2x_2 - 7x_3 = 8$ (2.35)
 $9x_1 + 5x_2 - 3x_3 = 2$

and use the rules for matrix multiplication, we can write this equation system in a more compact form as

$$\begin{bmatrix} 2 & 3 & 5 \\ 4 & -2 & -7 \\ 9 & 5 & -3 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 1 \\ 8 \\ 2 \end{bmatrix}.$$
 (2.36)

Note that x_1 scales the first column, x_2 the second one, and x_3 the third one.

Generally, a system of linear equations can be compactly represented in their matrix form as Ax = b; see (2.3), and the product Ax is a (linear) combination of the columns of A. We will discuss linear combinations in more detail in Section 2.5.

2.3 Solving Systems of Linear Equations

In (2.3), we introduced the general form of an equation system, i.e.,

$$a_{11}x_1 + \dots + a_{1n}x_n = b_1$$

$$\vdots$$

$$a_{m1}x_1 + \dots + a_{mn}x_n = b_m,$$
(2.37)

where $a_{ij} \in \mathbb{R}$ and $b_i \in \mathbb{R}$ are known constants and x_j are unknowns, $i=1,\ldots,m,\,j=1,\ldots,n$. Thus far, we saw that matrices can be used as a compact way of formulating systems of linear equations so that we can write Ax = b, see (2.10). Moreover, we defined basic matrix operations, such as addition and multiplication of matrices. In the following, we will focus on solving systems of linear equations and provide an algorithm for finding the inverse of a matrix.

2.3.1 Particular and General Solution

Before discussing how to generally solve systems of linear equations, let us have a look at an example. Consider the system of equations

$$\begin{bmatrix} 1 & 0 & 8 & -4 \\ 0 & 1 & 2 & 12 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 42 \\ 8 \end{bmatrix}.$$
 (2.38)

The system has two equations and four unknowns. Therefore, in general we would expect infinitely many solutions. This system of equations is in a particularly easy form, where the first two columns consist of a 1 and a 0. Remember that we want to find scalars x_1, \ldots, x_4 , such that $\sum_{i=1}^4 x_i c_i = b$, where we define c_i to be the ith column of the matrix and b the right-hand-side of (2.38). A solution to the problem in (2.38) can be found immediately by taking 42 times the first column and 8 times the second column so that

$$\boldsymbol{b} = \begin{bmatrix} 42\\8 \end{bmatrix} = 42 \begin{bmatrix} 1\\0 \end{bmatrix} + 8 \begin{bmatrix} 0\\1 \end{bmatrix}. \tag{2.39}$$

Therefore, a solution is $[42,8,0,0]^{\top}$. This solution is called a *particular solution* or *special solution*. However, this is not the only solution of this system of linear equations. To capture all the other solutions, we need to be creative in generating $\mathbf{0}$ in a non-trivial way using the columns of the matrix: Adding $\mathbf{0}$ to our special solution does not change the special solution. To do so, we express the third column using the first two columns (which are of this very simple form)

$$\begin{bmatrix} 8 \\ 2 \end{bmatrix} = 8 \begin{bmatrix} 1 \\ 0 \end{bmatrix} + 2 \begin{bmatrix} 0 \\ 1 \end{bmatrix} \tag{2.40}$$

so that $\mathbf{0} = 8\mathbf{c}_1 + 2\mathbf{c}_2 - 1\mathbf{c}_3 + 0\mathbf{c}_4$ and $(x_1, x_2, x_3, x_4) = (8, 2, -1, 0)$. In fact, any scaling of this solution by $\lambda_1 \in \mathbb{R}$ produces the $\mathbf{0}$ vector, i.e.,

$$\begin{bmatrix} 1 & 0 & 8 & -4 \\ 0 & 1 & 2 & 12 \end{bmatrix} \begin{pmatrix} \lambda_1 \begin{bmatrix} 8 \\ 2 \\ -1 \\ 0 \end{bmatrix} \end{pmatrix} = \lambda_1 (8\boldsymbol{c}_1 + 2\boldsymbol{c}_2 - \boldsymbol{c}_3) = \boldsymbol{0}.$$
 (2.41)

Following the same line of reasoning, we express the fourth column of the matrix in (2.38) using the first two columns and generate another set of non-trivial versions of $\mathbf{0}$ as

$$\begin{bmatrix} 1 & 0 & 8 & -4 \\ 0 & 1 & 2 & 12 \end{bmatrix} \begin{pmatrix} \lambda_2 \begin{bmatrix} -4 \\ 12 \\ 0 \\ -1 \end{bmatrix} \end{pmatrix} = \lambda_2 (-4\boldsymbol{c}_1 + 12\boldsymbol{c}_2 - \boldsymbol{c}_4) = \boldsymbol{0}$$
 (2.42)

for any $\lambda_2 \in \mathbb{R}$. Putting everything together, we obtain all solutions of the general solution equation system in (2.38), which is called the *general solution*, as the set

 $\left\{ \boldsymbol{x} \in \mathbb{R}^4 : \boldsymbol{x} = \begin{bmatrix} 42 \\ 8 \\ 0 \\ 0 \end{bmatrix} + \lambda_1 \begin{bmatrix} 8 \\ 2 \\ -1 \\ 0 \end{bmatrix} + \lambda_2 \begin{bmatrix} -4 \\ 12 \\ 0 \\ -1 \end{bmatrix}, \lambda_1, \lambda_2 \in \mathbb{R} \right\}. \quad (2.43)$

Remark. The general approach we followed consisted of the following three steps:

- 1. Find a particular solution to Ax = b.
- 2. Find all solutions to Ax = 0.
- 3. Combine the solutions from steps 1. and 2. to the general solution.

 \Diamond

Neither the general nor the particular solution is unique.

The system of linear equations in the preceding example was easy to solve because the matrix in (2.38) has this particularly convenient form, which allowed us to find the particular and the general solution by inspection. However, general equation systems are not of this simple form. Fortunately, there exists a constructive algorithmic way of transforming any system of linear equations into this particularly simple form: Gaussian elimination. Key to Gaussian elimination are elementary transformations of systems of linear equations, which transform the equation system into a simple form. Then, we can apply the three steps to the simple form that we just discussed in the context of the example in (2.38).

2.3.2 Elementary Transformations

elementary transformations Key to solving a system of linear equations are *elementary transformations* that keep the solution set the same, but that transform the equation system into a simpler form:

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- Exchange of two equations (rows in the matrix representing the system of equations)
- Multiplication of an equation (row) with a constant $\lambda \in \mathbb{R} \setminus \{0\}$
- Addition of two equations (rows)

Example 2.6

For $a \in \mathbb{R}$, we seek all solutions of the following system of equations:

We start by converting this system of equations into the compact matrix notation Ax = b. We no longer mention the variables x explicitly and build the *augmented matrix* (in the form $\begin{bmatrix} A \mid b \end{bmatrix}$)

augmented matrix

$$\left[\begin{array}{ccc|ccc|c} -2 & 4 & -2 & -1 & 4 & -3 \\ 4 & -8 & 3 & -3 & 1 & 2 \\ 1 & -2 & 1 & -1 & 1 & 0 \\ 1 & -2 & 0 & -3 & 4 & a \end{array} \right] \text{ Swap with } R_1$$

where we used the vertical line to separate the left-hand side from the right-hand side in (2.44). We use \leadsto to indicate a transformation of the augmented matrix using elementary transformations.

Swapping Rows 1 and 3 leads to

$$\begin{bmatrix} 1 & -2 & 1 & -1 & 1 & 0 \\ 4 & -8 & 3 & -3 & 1 & 2 \\ -2 & 4 & -2 & -1 & 4 & -3 \\ 1 & -2 & 0 & -3 & 4 & a \end{bmatrix} -4R_1 +2R_1$$

When we now apply the indicated transformations (e.g., subtract Row 1 four times from Row 2), we obtain

The augmented matrix $\begin{bmatrix} A \mid b \end{bmatrix}$ compactly represents the system of linear equations Ax = b.

row-echelon form

This (augmented) matrix is in a convenient form, the *row-echelon form* (REF). Reverting this compact notation back into the explicit notation with the variables we seek, we obtain

particular solution

Only for a = -1 this system can be solved. A particular solution is

$$\begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \\ x_5 \end{bmatrix} = \begin{bmatrix} 2 \\ 0 \\ -1 \\ 1 \\ 0 \end{bmatrix} . \tag{2.46}$$

general solution

The general solution, which captures the set of all possible solutions, is

$$\left\{ \boldsymbol{x} \in \mathbb{R}^5 : \boldsymbol{x} = \begin{bmatrix} 2\\0\\-1\\1\\0 \end{bmatrix} + \lambda_1 \begin{bmatrix} 2\\1\\0\\0\\0 \end{bmatrix} + \lambda_2 \begin{bmatrix} 2\\0\\-1\\2\\1 \end{bmatrix}, \quad \lambda_1, \lambda_2 \in \mathbb{R} \right\}.$$
(2.47)

In the following, we will detail a constructive way to obtain a particular and general solution of a system of linear equations.

Remark (Pivots and Staircase Structure). The leading coefficient of a row (first nonzero number from the left) is called the *pivot* and is always strictly to the right of the pivot of the row above it. Therefore, any equation system in row-echelon form always has a "staircase" structure.

pivot

row-echelon form

Definition 2.6 (Row-Echelon Form). A matrix is in row-echelon form if

- All rows that contain only zeros are at the bottom of the matrix; correspondingly, all rows that contain at least one nonzero element are on top of rows that contain only zeros.
- Looking at nonzero rows only, the first nonzero number from the left (also called the *pivot* or the *leading coefficient*) is always strictly to the right of the pivot of the row above it.

Remark (Basic and Free Variables). The variables corresponding to the pivots in the row-echelon form are called *basic variables* and the other variables are *free variables*. For example, in (2.45), x_1, x_3, x_4 are basic variables, whereas x_2, x_5 are free variables. \diamondsuit

Remark (Obtaining a Particular Solution). The row-echelon form makes

pivot leading coefficient In other texts, it is sometimes required that the pivot is 1. basic variable free variable

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our lives easier when we need to determine a particular solution. To do this, we express the right-hand side of the equation system using the pivot columns, such that $\boldsymbol{b} = \sum_{i=1}^P \lambda_i \boldsymbol{p}_i$, where \boldsymbol{p}_i , $i=1,\ldots,P$, are the pivot columns. The λ_i are determined easiest if we start with the rightmost pivot column and work our way to the left.

In the previous example, we would try to find $\lambda_1, \lambda_2, \lambda_3$ so that

$$\lambda_{1} \begin{bmatrix} 1\\0\\0\\0\\0 \end{bmatrix} + \lambda_{2} \begin{bmatrix} 1\\1\\0\\0 \end{bmatrix} + \lambda_{3} \begin{bmatrix} -1\\-1\\1\\0 \end{bmatrix} = \begin{bmatrix} 0\\-2\\1\\0 \end{bmatrix}. \tag{2.48}$$

From here, we find relatively directly that $\lambda_3 = 1, \lambda_2 = -1, \lambda_1 = 2$. When we put everything together, we must not forget the non-pivot columns for which we set the coefficients implicitly to 0. Therefore, we get the particular solution $\boldsymbol{x} = [2, 0, -1, 1, 0]^{\top}$.

Remark (Reduced Row Echelon Form). An equation system is in reduced row-echelon form (also: row-reduced echelon form or row canonical form) if

reduced row-echelon form

- It is in row-echelon form.
- Every pivot is 1.
- The pivot is the only nonzero entry in its column.

 \Diamond

The reduced row-echelon form will play an important role later in Section 2.3.3 because it allows us to determine the general solution of a system of linear equations in a straightforward way.

Remark (Gaussian Elimination). Gaussian elimination is an algorithm that performs elementary transformations to bring a system of linear equations into reduced row-echelon form.

Gaussian elimination

Example 2.7 (Reduced Row Echelon Form)

Verify that the following matrix is in reduced row-echelon form (the pivots are in **bold**):

$$\mathbf{A} = \begin{bmatrix} \mathbf{1} & 3 & 0 & 0 & 3 \\ 0 & 0 & \mathbf{1} & 0 & 9 \\ 0 & 0 & 0 & \mathbf{1} & -4 \end{bmatrix} . \tag{2.49}$$

The key idea for finding the solutions of Ax = 0 is to look at the *non-pivot columns*, which we will need to express as a (linear) combination of the pivot columns. The reduced row echelon form makes this relatively straightforward, and we express the non-pivot columns in terms of sums and multiples of the pivot columns that are on their left: The second column is 3 times the first column (we can ignore the pivot columns on the right of the second column). Therefore, to obtain $\mathbf{0}$, we need to subtract

the second column from three times the first column. Now, we look at the fifth column, which is our second non-pivot column. The fifth column can be expressed as 3 times the first pivot column, 9 times the second pivot column, and -4 times the third pivot column. We need to keep track of the indices of the pivot columns and translate this into 3 times the first column, 0 times the second column (which is a non-pivot column), 9 times the third column (which is our second pivot column), and -4 times the fourth column (which is the third pivot column). Then we need to subtract the fifth column to obtain 0. In the end, we are still solving a homogeneous equation system.

To summarize, all solutions of $Ax=\mathbf{0}, x\in\mathbb{R}^5$ are given by

$$\left\{ \boldsymbol{x} \in \mathbb{R}^5 : \boldsymbol{x} = \lambda_1 \begin{bmatrix} 3 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \lambda_2 \begin{bmatrix} 3 \\ 0 \\ 9 \\ -4 \\ -1 \end{bmatrix}, \quad \lambda_1, \lambda_2 \in \mathbb{R} \right\}.$$
(2.50)

2.3.3 The Minus-1 Trick

In the following, we introduce a practical trick for reading out the solutions x of a homogeneous system of linear equations Ax = 0, where $A \in \mathbb{R}^{k \times n}$, $x \in \mathbb{R}^n$.

To start, we assume that A is in reduced row-echelon form without any rows that just contain zeros, i.e.,

where * can be an arbitrary real number, with the constraints that the first nonzero entry per row must be 1 and all other entries in the corresponding column must be 0. The columns j_1,\ldots,j_k with the pivots (marked in **bold**) are the standard unit vectors $\boldsymbol{e}_1,\ldots,\boldsymbol{e}_k\in\mathbb{R}^k$. We extend this matrix to an $n\times n$ -matrix $\tilde{\boldsymbol{A}}$ by adding n-k rows of the form

$$\begin{bmatrix} 0 & \cdots & 0 & -1 & 0 & \cdots & 0 \end{bmatrix} \tag{2.52}$$

so that the diagonal of the augmented matrix \tilde{A} contains either 1 or -1. Then, the columns of \tilde{A} that contain the -1 as pivots are solutions of

the homogeneous equation system Ax = 0. To be more precise, these columns form a basis (Section 2.6.1) of the solution space of Ax = 0, which we will later call the *kernel* or *null space* (see Section 2.7.3).

kernel null space

Example 2.8 (Minus-1 Trick)

Let us revisit the matrix in (2.49), which is already in reduced REF:

$$\mathbf{A} = \begin{bmatrix} 1 & 3 & 0 & 0 & 3 \\ 0 & 0 & 1 & 0 & 9 \\ 0 & 0 & 0 & 1 & -4 \end{bmatrix} . \tag{2.53}$$

We now augment this matrix to a 5×5 matrix by adding rows of the form (2.52) at the places where the pivots on the diagonal are missing and obtain

$$\tilde{\mathbf{A}} = \begin{bmatrix} 1 & 3 & 0 & 0 & 3 \\ 0 & -\mathbf{1} & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 9 \\ 0 & 0 & 0 & 1 & -4 \\ 0 & 0 & 0 & 0 & -\mathbf{1} \end{bmatrix} . \tag{2.54}$$

From this form, we can immediately read out the solutions of Ax = 0 by taking the columns of \tilde{A} , which contain -1 on the diagonal:

$$\left\{ \boldsymbol{x} \in \mathbb{R}^5 : \boldsymbol{x} = \lambda_1 \begin{bmatrix} 3 \\ -1 \\ 0 \\ 0 \\ 0 \end{bmatrix} + \lambda_2 \begin{bmatrix} 3 \\ 0 \\ 9 \\ -4 \\ -1 \end{bmatrix}, \quad \lambda_1, \lambda_2 \in \mathbb{R} \right\},$$
(2.55)

which is identical to the solution in (2.50) that we obtained by "insight".

Calculating the Inverse

To compute the inverse A^{-1} of $A \in \mathbb{R}^{n \times n}$, we need to find a matrix X that satisfies $AX = I_n$. Then, $X = A^{-1}$. We can write this down as a set of simultaneous linear equations $AX = I_n$, where we solve for $X = [x_1|\cdots|x_n]$. We use the augmented matrix notation for a compact representation of this set of systems of linear equations and obtain

$$[A|I_n] \longrightarrow \cdots \longrightarrow [I_n|A^{-1}].$$
 (2.56)

This means that if we bring the augmented equation system into reduced row-echelon form, we can read out the inverse on the right-hand side of the equation system. Hence, determining the inverse of a matrix is equivalent to solving systems of linear equations. Example 2.9 (Calculating an Inverse Matrix by Gaussian Elimination)
To determine the inverse of

$$\mathbf{A} = \begin{bmatrix} 1 & 0 & 2 & 0 \\ 1 & 1 & 0 & 0 \\ 1 & 2 & 0 & 1 \\ 1 & 1 & 1 & 1 \end{bmatrix} \tag{2.57}$$

we write down the augmented matrix

$$\begin{bmatrix}
1 & 0 & 2 & 0 & 1 & 0 & 0 & 0 \\
1 & 1 & 0 & 0 & 0 & 1 & 0 & 0 \\
1 & 2 & 0 & 1 & 0 & 0 & 1 & 0 \\
1 & 1 & 1 & 1 & 0 & 0 & 0 & 1
\end{bmatrix}$$

and use Gaussian elimination to bring it into reduced row-echelon form

$$\begin{bmatrix} 1 & 0 & 0 & 0 & | & -1 & 2 & -2 & 2 \\ 0 & 1 & 0 & 0 & | & 1 & -1 & 2 & -2 \\ 0 & 0 & 1 & 0 & | & 1 & -1 & 1 & -1 \\ 0 & 0 & 0 & 1 & | & -1 & 0 & -1 & 2 \end{bmatrix},$$

such that the desired inverse is given as its right-hand side:

$$\mathbf{A}^{-1} = \begin{bmatrix} -1 & 2 & -2 & 2\\ 1 & -1 & 2 & -2\\ 1 & -1 & 1 & -1\\ -1 & 0 & -1 & 2 \end{bmatrix} . \tag{2.58}$$

We can verify that (2.58) is indeed the inverse by performing the multiplication AA^{-1} and observing that we recover I_4 .

2.3.4 Algorithms for Solving a System of Linear Equations

In the following, we briefly discuss approaches to solving a system of linear equations of the form Ax = b. We make the assumption that a solution exists. Should there be no solution, we need to resort to approximate solutions, which we do not cover in this chapter. One way to solve the approximate problem is using the approach of linear regression, which we discuss in detail in Chapter 9.

In special cases, we may be able to determine the inverse A^{-1} , such that the solution of Ax = b is given as $x = A^{-1}b$. However, this is only possible if A is a square matrix and invertible, which is often not the case. Otherwise, under mild assumptions (i.e., A needs to have linearly independent columns) we can use the transformation

$$Ax = b \iff A^{\top}Ax = A^{\top}b \iff x = (A^{\top}A)^{-1}A^{\top}b$$
 (2.59)

and use the *Moore-Penrose pseudo-inverse* $(A^{\top}A)^{-1}A^{\top}$ to determine the solution (2.59) that solves Ax = b, which also corresponds to the minimum norm least-squares solution. A disadvantage of this approach is that it requires many computations for the matrix-matrix product and computing the inverse of $A^{\top}A$. Moreover, for reasons of numerical precision it is generally not recommended to compute the inverse or pseudo-inverse. In the following, we therefore briefly discuss alternative approaches to solving systems of linear equations.

Gaussian elimination plays an important role when computing determinants (Section 4.1), checking whether a set of vectors is linearly independent (Section 2.5), computing the inverse of a matrix (Section 2.2.2), computing the rank of a matrix (Section 2.6.2), and determining a basis of a vector space (Section 2.6.1). Gaussian elimination is an intuitive and constructive way to solve a system of linear equations with thousands of variables. However, for systems with millions of variables, it is impractical as the required number of arithmetic operations scales cubically in the number of simultaneous equations.

In practice, systems of many linear equations are solved indirectly, by either stationary iterative methods, such as the Richardson method, the Jacobi method, the Gauß-Seidel method, and the successive over-relaxation method, or Krylov subspace methods, such as conjugate gradients, generalized minimal residual, or biconjugate gradients. We refer to the books by Stoer and Burlirsch (2002), Strang (2003), and Liesen and Mehrmann (2015) for further details.

Let x_* be a solution of Ax = b. The key idea of these iterative methods is to set up an iteration of the form

$$x^{(k+1)} = Cx^{(k)} + d (2.60)$$

for suitable C and d that reduces the residual error $\|x^{(k+1)} - x_*\|$ in every iteration and converges to x_* . We will introduce norms $\|\cdot\|$, which allow us to compute similarities between vectors, in Section 3.1.

2.4 Vector Spaces

Thus far, we have looked at systems of linear equations and how to solve them (Section 2.3). We saw that systems of linear equations can be compactly represented using matrix-vector notation (2.10). In the following, we will have a closer look at vector spaces, i.e., a structured space in which vectors live.

In the beginning of this chapter, we informally characterized vectors as objects that can be added together and multiplied by a scalar, and they remain objects of the same type. Now, we are ready to formalize this, and we will start by introducing the concept of a group, which is a set of elements and an operation defined on these elements that keeps some structure of the set intact.

2.4.1 Groups

Groups play an important role in computer science. Besides providing a fundamental framework for operations on sets, they are heavily used in cryptography, coding theory, and graphics.

Definition 2.7 (Group). Consider a set \mathcal{G} and an operation $\otimes : \mathcal{G} \times \mathcal{G} \to \mathcal{G}$ defined on \mathcal{G} . Then $G := (\mathcal{G}, \otimes)$ is called a *group* if the following hold:

group closure associativity neutral element inverse element

- 1. Closure of \mathcal{G} under \otimes : $\forall x, y \in \mathcal{G} : x \otimes y \in \mathcal{G}$
- 2. Associativity: $\forall x, y, z \in \mathcal{G} : (x \otimes y) \otimes z = x \otimes (y \otimes z)$
- 3. Neutral element: $\exists e \in \mathcal{G} \ \forall x \in \mathcal{G} : x \otimes e = x \text{ and } e \otimes x = x$
- 4. Inverse element: $\forall x \in \mathcal{G} \exists y \in \mathcal{G} : x \otimes y = e \text{ and } y \otimes x = e, \text{ where } e \text{ is}$ the neutral element. We often write x^{-1} to denote the inverse element of x.

Remark. The inverse element is defined with respect to the operation \otimes and does not necessarily mean $\frac{1}{x}$.

Abelian group

If additionally $\forall x, y \in \mathcal{G} : x \otimes y = y \otimes x$, then $G = (\mathcal{G}, \otimes)$ is an Abelian group (commutative).

Example 2.10 (Groups)

Let us have a look at some examples of sets with associated operations and see whether they are groups:

• $(\mathbb{Z}, +)$ is an Abelian group.

• $(\mathbb{N}_0,+)$ is not a group: Although $(\mathbb{N}_0,+)$ possesses a neutral element (0), the inverse elements are missing.

- (\mathbb{Z},\cdot) is not a group: Although (\mathbb{Z},\cdot) contains a neutral element (1), the inverse elements for any $z \in \mathbb{Z}, z \neq \pm 1$, are missing.
- (\mathbb{R},\cdot) is not a group since 0 does not possess an inverse element.
- $(\mathbb{R}\setminus\{0\},\cdot)$ is Abelian.
- $(\mathbb{R}^n, +), (\mathbb{Z}^n, +), n \in \mathbb{N}$ are Abelian if + is defined componentwise, i.e.,

$$(x_1, \dots, x_n) + (y_1, \dots, y_n) = (x_1 + y_1, \dots, x_n + y_n).$$
 (2.61)

Then, $(x_1, \dots, x_n)^{-1} := (-x_1, \dots, -x_n)$ is the inverse element and $e = (0, \cdots, 0)$ is the neutral element.

- $(\mathbb{R}^{m \times n}, +)$, the set of $m \times n$ -matrices is Abelian (with componentwise addition as defined in (2.61)).
- Let us have a closer look at $(\mathbb{R}^{n\times n},\cdot)$, i.e., the set of $n\times n$ -matrices with matrix multiplication as defined in (2.13).
 - Closure and associativity follow directly from the definition of matrix multiplication.
 - Neutral element: The identity matrix I_n is the neutral element with respect to matrix multiplication " \cdot " in $(\mathbb{R}^{n \times n}, \cdot)$.

 $\mathbb{N}_0 := \mathbb{N} \cup \{0\}$

– Inverse element: If the inverse exists (A is regular), then A^{-1} is the inverse element of $A \in \mathbb{R}^{n \times n}$, and in exactly this case $(\mathbb{R}^{n \times n}, \cdot)$ is a group, called the *general linear group*.

Definition 2.8 (General Linear Group). The set of regular (invertible) matrices $A \in \mathbb{R}^{n \times n}$ is a group with respect to matrix multiplication as defined in (2.13) and is called *general linear group* $GL(n,\mathbb{R})$. However, since matrix multiplication is not commutative, the group is not Abelian.

general linear group

2.4.2 Vector Spaces

When we discussed groups, we looked at sets $\mathcal G$ and inner operations on $\mathcal G$, i.e., mappings $\mathcal G \times \mathcal G \to \mathcal G$ that only operate on elements in $\mathcal G$. In the following, we will consider sets that in addition to an inner operation + also contain an outer operation \cdot , the multiplication of a vector $x \in \mathcal G$ by a scalar $\lambda \in \mathbb R$. We can think of the inner operation as a form of addition, and the outer operation as a form of scaling. Note that the inner/outer operations have nothing to do with inner/outer products.

Definition 2.9 (Vector Space). A real-valued *vector space* $V = (V, +, \cdot)$ is vector space a set V with two operations

$$+: \mathcal{V} \times \mathcal{V} \to \mathcal{V}$$
 (2.62)

$$\cdot: \ \mathbb{R} \times \mathcal{V} \to \mathcal{V} \tag{2.63}$$

where

- 1. $(\mathcal{V}, +)$ is an Abelian group
- 2. Distributivity:

1.
$$\forall \lambda \in \mathbb{R}, \boldsymbol{x}, \boldsymbol{y} \in \mathcal{V} : \lambda \cdot (\boldsymbol{x} + \boldsymbol{y}) = \lambda \cdot \boldsymbol{x} + \lambda \cdot \boldsymbol{y}$$

2.
$$\forall \lambda, \psi \in \mathbb{R}, \boldsymbol{x} \in \mathcal{V} : (\lambda + \psi) \cdot \boldsymbol{x} = \lambda \cdot \boldsymbol{x} + \psi \cdot \boldsymbol{x}$$

- 3. Associativity (outer operation): $\forall \lambda, \psi \in \mathbb{R}, x \in \mathcal{V} : \lambda \cdot (\psi \cdot x) = (\lambda \psi) \cdot x$
- 4. Neutral element with respect to the outer operation: $\forall x \in \mathcal{V} : 1 \cdot x = x$

The elements $x \in V$ are called *vectors*. The neutral element of $(\mathcal{V}, +)$ is the zero vector $\mathbf{0} = [0, \dots, 0]^{\mathsf{T}}$, and the inner operation + is called *vector addition*. The elements $\lambda \in \mathbb{R}$ are called *scalars* and the outer operation \cdot is a *multiplication by scalars*. Note that a scalar product is something different, and we will get to this in Section 3.2.

vector vector addition scalar multiplication by scalars

Remark. A "vector multiplication" ab, a, $b \in \mathbb{R}^n$, is not defined. Theoretically, we could define an element-wise multiplication, such that c=ab with $c_j=a_jb_j$. This "array multiplication" is common to many programming languages but makes mathematically limited sense using the standard rules for matrix multiplication: By treating vectors as $n \times 1$ matrices

outer product

(which we usually do), we can use the matrix multiplication as defined in (2.13). However, then the dimensions of the vectors do not match. Only the following multiplications for vectors are defined: $ab^{\perp} \in \mathbb{R}^{n \times n}$ (outer product), $a^{\top}b \in \mathbb{R}$ (inner/scalar/dot product).

Example 2.11 (Vector Spaces)

Let us have a look at some important examples:

- $\mathcal{V} = \mathbb{R}^n, n \in \mathbb{N}$ is a vector space with operations defined as follows:
 - Addition: $x+y=(x_1,\ldots,x_n)+(y_1,\ldots,y_n)=(x_1+y_1,\ldots,x_n+y_n)$ for all $\boldsymbol{x}, \boldsymbol{y} \in \mathbb{R}^n$
 - Multiplication by scalars: $\lambda x = \lambda(x_1, \dots, x_n) = (\lambda x_1, \dots, \lambda x_n)$ for all $\lambda \in \mathbb{R}, \boldsymbol{x} \in \mathbb{R}^n$
- $\mathcal{V} = \mathbb{R}^{m \times n}, m, n \in \mathbb{N}$ is a vector space with
- Addition: $m{A} + m{B} = \begin{bmatrix} a_{11} + b_{11} & \cdots & a_{1n} + b_{1n} \\ \vdots & & \vdots \\ a_{m1} + b_{m1} & \cdots & a_{mn} + b_{mn} \end{bmatrix}$ is defined elementwise for all $m{A}, m{B} \in \mathcal{V}$
 - Multiplication by scalars: $\lambda A = \begin{bmatrix} \lambda a_{11} & \cdots & \lambda a_{1n} \\ \vdots & & \vdots \\ \lambda a_{m1} & \cdots & \lambda a_{mn} \end{bmatrix}$ as defined in

Section 2.2. Remember that $\mathbb{R}^{m \times n}$ is equivalent to \mathbb{R}

• $\mathcal{V} = \mathbb{C}$, with the standard definition of addition of complex numbers.

Remark. In the following, we will denote a vector space $(\mathcal{V}, +, \cdot)$ by V when + and \cdot are the standard vector addition and scalar multiplication. Moreover, we will use the notation $x \in V$ for vectors in \mathcal{V} to simplify notation.

Remark. The vector spaces \mathbb{R}^n , $\mathbb{R}^{n\times 1}$, $\mathbb{R}^{1\times n}$ are only different in the way we write vectors. In the following, we will not make a distinction between \mathbb{R}^n and $\mathbb{R}^{n\times 1}$, which allows us to write *n*-tuples as *column vectors*

column vector

$$x = \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} . \tag{2.64}$$

row vector

transpose

This simplifies the notation regarding vector space operations. However, we do distinguish between $\mathbb{R}^{n\times 1}$ and $\mathbb{R}^{1\times n}$ (the *row vectors*) to avoid confusion with matrix multiplication. By default, we write x to denote a column vector, and a row vector is denoted by x^{\top} , the *transpose* of x.

2.4.3 Vector Subspaces

In the following, we will introduce vector subspaces. Intuitively, they are sets contained in the original vector space with the property that when we perform vector space operations on elements within this subspace, we will never leave it. In this sense, they are "closed". Vector subspaces are a key idea in machine learning. For example, Chapter 10 demonstrates how to use vector subspaces for dimensionality reduction.

Definition 2.10 (Vector Subspace). Let $V=(\mathcal{V},+,\cdot)$ be a vector space and $\mathcal{U}\subseteq\mathcal{V},\,\mathcal{U}\neq\emptyset$. Then $U=(\mathcal{U},+,\cdot)$ is called *vector subspace* of V (or *linear subspace*) if U is a vector space with the vector space operations + and \cdot restricted to $\mathcal{U}\times\mathcal{U}$ and $\mathbb{R}\times\mathcal{U}$. We write $U\subseteq V$ to denote a subspace U of V.

vector subspace linear subspace

If $\mathcal{U}\subseteq\mathcal{V}$ and V is a vector space, then U naturally inherits many properties directly from V because they hold for all $\boldsymbol{x}\in\mathcal{V}$, and in particular for all $\boldsymbol{x}\in\mathcal{U}\subseteq\mathcal{V}$. This includes the Abelian group properties, the distributivity, the associativity and the neutral element. To determine whether $(\mathcal{U},+,\cdot)$ is a subspace of V we still do need to show

- 1. $\mathcal{U} \neq \emptyset$, in particular: $\mathbf{0} \in \mathcal{U}$
- 2. Closure of U:
 - a. With respect to the outer operation: $\forall \lambda \in \mathbb{R} \ \forall x \in \mathcal{U} : \lambda x \in \mathcal{U}$.
 - b. With respect to the inner operation: $\forall x, y \in \mathcal{U} : x + y \in \mathcal{U}$.

Example 2.12 (Vector Subspaces)

Let us have a look at some examples:

- For every vector space V, the trivial subspaces are V itself and $\{0\}$.
- Only example D in Figure 2.6 is a subspace of \mathbb{R}^2 (with the usual inner/outer operations). In A and C, the closure property is violated; B does not contain $\mathbf{0}$.
- The solution set of a homogeneous system of linear equations Ax = 0 with n unknowns $x = [x_1, \dots, x_n]^{\top}$ is a subspace of \mathbb{R}^n .
- The solution of an inhomogeneous system of linear equations Ax = b, $b \neq 0$ is not a subspace of \mathbb{R}^n .
- The intersection of arbitrarily many subspaces is a subspace itself.

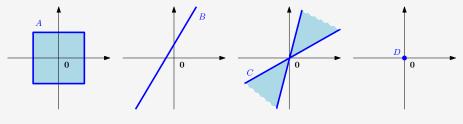


Figure 2.6 Not all subsets of \mathbb{R}^2 are subspaces. In A and C, the closure property is violated; B does not contain 0. Only D is a subspace.

Remark. Every subspace $U \subseteq (\mathbb{R}^n, +, \cdot)$ is the solution space of a homogeneous system of linear equations Ax = 0 for $x \in \mathbb{R}^n$.

2.5 Linear Independence

In the following, we will have a close look at what we can do with vectors (elements of the vector space). In particular, we can add vectors together and multiply them with scalars. The closure property guarantees that we end up with another vector in the same vector space. It is possible to find a set of vectors with which we can represent every vector in the vector space by adding them together and scaling them. This set of vectors is a *basis*, and we will discuss them in Section 2.6.1. Before we get there, we will need to introduce the concepts of linear combinations and linear independence.

Definition 2.11 (Linear Combination). Consider a vector space V and a finite number of vectors $x_1, \ldots, x_k \in V$. Then, every $v \in V$ of the form

$$oldsymbol{v} = \lambda_1 oldsymbol{x}_1 + \dots + \lambda_k oldsymbol{x}_k = \sum_{i=1}^k \lambda_i oldsymbol{x}_i \in V$$
 (2.65)

linear combination

with $\lambda_1, \ldots, \lambda_k \in \mathbb{R}$ is a linear combination of the vectors x_1, \ldots, x_k .

The **0**-vector can always be written as the linear combination of k vectors x_1, \ldots, x_k because $\mathbf{0} = \sum_{i=1}^k 0 x_i$ is always true. In the following, we are interested in non-trivial linear combinations of a set of vectors to represent $\mathbf{0}$, i.e., linear combinations of vectors x_1, \ldots, x_k , where not all coefficients λ_i in (2.65) are 0.

Definition 2.12 (Linear (In)dependence). Let us consider a vector space V with $k \in \mathbb{N}$ and $x_1, \ldots, x_k \in V$. If there is a non-trivial linear combination, such that $\mathbf{0} = \sum_{i=1}^k \lambda_i x_i$ with at least one $\lambda_i \neq 0$, the vectors x_1, \ldots, x_k are linearly dependent. If only the trivial solution exists, i.e., $\lambda_1 = \ldots = \lambda_k = 0$ the vectors x_1, \ldots, x_k are linearly independent.

linearly dependent linearly independent

Linear independence is one of the most important concepts in linear algebra. Intuitively, a set of linearly independent vectors consists of vectors that have no redundancy, i.e., if we remove any of those vectors from the set, we will lose something. Throughout the next sections, we will formalize this intuition more.

Example 2.13 (Linearly Dependent Vectors)

A geographic example may help to clarify the concept of linear independence. A person in Nairobi (Kenya) describing where Kigali (Rwanda) is might say ,"You can get to Kigali by first going $506\,\mathrm{km}$ Northwest to Kampala (Uganda) and then $374\,\mathrm{km}$ Southwest.". This is sufficient information

to describe the location of Kigali because the geographic coordinate system may be considered a two-dimensional vector space (ignoring altitude and the Earth's curved surface). The person may add, "It is about $751\,\mathrm{km}$ West of here." Although this last statement is true, it is not necessary to find Kigali given the previous information (see Figure 2.7 for an illustration). In this example, the " $506\,\mathrm{km}$ Northwest" vector (blue) and the " $374\,\mathrm{km}$ Southwest" vector (purple) are linearly independent. This means the Southwest vector cannot be described in terms of the Northwest vector, and vice versa. However, the third " $751\,\mathrm{km}$ West" vector (black) is a linear combination of the other two vectors, and it makes the set of vectors linearly dependent. Equivalently, given " $751\,\mathrm{km}$ West" and " $374\,\mathrm{km}$ Southwest" can be linearly combined to obtain " $506\,\mathrm{km}$ Northwest".

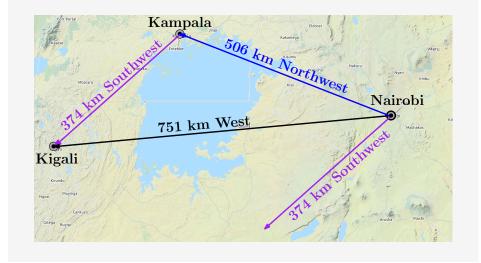


Figure 2.7
Geographic example
(with crude
approximations to
cardinal directions)
of linearly
dependent vectors
in a
two-dimensional
space (plane).

Remark. The following properties are useful to find out whether vectors are linearly independent:

- *k* vectors are either linearly dependent or linearly independent. There is no third option.
- If at least one of the vectors x_1, \dots, x_k is $\mathbf{0}$ then they are linearly dependent. The same holds if two vectors are identical.
- The vectors $\{x_1, \ldots, x_k : x_i \neq \mathbf{0}, i = 1, \ldots, k\}$, $k \geqslant 2$, are linearly dependent if and only if (at least) one of them is a linear combination of the others. In particular, if one vector is a multiple of another vector, i.e., $x_i = \lambda x_j$, $\lambda \in \mathbb{R}$ then the set $\{x_1, \ldots, x_k : x_i \neq \mathbf{0}, i = 1, \ldots, k\}$ is linearly dependent.
- A practical way of checking whether vectors $x_1, ..., x_k \in V$ are linearly independent is to use Gaussian elimination: Write all vectors as columns of a matrix A and perform Gaussian elimination until the matrix is in row echelon form (the reduced row-echelon form is unnecessary here):

The pivot columns indicate the vectors, which are linearly independent of the vectors on the left. Note that there is an ordering of vectors when the matrix is built.

 The non-pivot columns can be expressed as linear combinations of the pivot columns on their left. For instance, the row-echelon form

$$\begin{bmatrix} 1 & 3 & 0 \\ 0 & 0 & 2 \end{bmatrix} \tag{2.66}$$

tells us that the first and third columns are pivot columns. The second column is a non-pivot column because it is three times the first column.

All column vectors are linearly independent if and only if all columns are pivot columns. If there is at least one non-pivot column, the columns (and, therefore, the corresponding vectors) are linearly dependent.



Example 2.14

Consider \mathbb{R}^4 with

$$x_1 = \begin{bmatrix} 1 \\ 2 \\ -3 \\ 4 \end{bmatrix}, \quad x_2 = \begin{bmatrix} 1 \\ 1 \\ 0 \\ 2 \end{bmatrix}, \quad x_3 = \begin{bmatrix} -1 \\ -2 \\ 1 \\ 1 \end{bmatrix}.$$
 (2.67)

To check whether they are linearly dependent, we follow the general approach and solve

$$\lambda_1 \boldsymbol{x}_1 + \lambda_2 \boldsymbol{x}_2 + \lambda_3 \boldsymbol{x}_3 = \lambda_1 \begin{bmatrix} 1\\2\\-3\\4 \end{bmatrix} + \lambda_2 \begin{bmatrix} 1\\1\\0\\2 \end{bmatrix} + \lambda_3 \begin{bmatrix} -1\\-2\\1\\1 \end{bmatrix} = \boldsymbol{0} \qquad (2.68)$$

for $\lambda_1, \ldots, \lambda_3$. We write the vectors \boldsymbol{x}_i , i=1,2,3, as the columns of a matrix and apply elementary row operations until we identify the pivot columns:

$$\begin{bmatrix} 1 & 1 & -1 \\ 2 & 1 & -2 \\ -3 & 0 & 1 \\ 4 & 2 & 1 \end{bmatrix} \longrightarrow \cdots \longrightarrow \begin{bmatrix} 1 & 1 & -1 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{bmatrix}. \tag{2.69}$$

Here, every column of the matrix is a pivot column. Therefore, there is no non-trivial solution, and we require $\lambda_1=0, \lambda_2=0, \lambda_3=0$ to solve the equation system. Hence, the vectors $\boldsymbol{x}_1, \boldsymbol{x}_2, \boldsymbol{x}_3$ are linearly independent.

Remark. Consider a vector space V with k linearly independent vectors $\mathbf{b}_1, \dots, \mathbf{b}_k$ and m linear combinations

$$egin{aligned} oldsymbol{x}_1 &= \sum_{i=1}^k \lambda_{i1} oldsymbol{b}_i \,, \ &dots \ oldsymbol{x}_m &= \sum_{i=1}^k \lambda_{im} oldsymbol{b}_i \,. \end{aligned}$$

Defining $B = [b_1, ..., b_k]$ as the matrix whose columns are the linearly independent vectors $b_1, ..., b_k$, we can write

$$\boldsymbol{x}_{j} = \boldsymbol{B}\boldsymbol{\lambda}_{j}, \quad \boldsymbol{\lambda}_{j} = \begin{bmatrix} \lambda_{1j} \\ \vdots \\ \lambda_{kj} \end{bmatrix}, \quad j = 1, \dots, m,$$
 (2.71)

in a more compact form.

We want to test whether x_1, \ldots, x_m are linearly independent. For this purpose, we follow the general approach of testing when $\sum_{j=1}^m \psi_j x_j = \mathbf{0}$. With (2.71), we obtain

$$\sum_{j=1}^{m} \psi_j \boldsymbol{x}_j = \sum_{j=1}^{m} \psi_j \boldsymbol{B} \boldsymbol{\lambda}_j = \boldsymbol{B} \sum_{j=1}^{m} \psi_j \boldsymbol{\lambda}_j.$$
 (2.72)

This means that $\{x_1, \dots, x_m\}$ are linearly independent if and only if the column vectors $\{\lambda_1, \dots, \lambda_m\}$ are linearly independent.

 \Diamond

Remark. In a vector space V, m linear combinations of k vectors $\mathbf{x}_1, \dots, \mathbf{x}_k$ are linearly dependent if m > k.

Example 2.15

Consider a set of linearly independent vectors $\boldsymbol{b}_1, \boldsymbol{b}_2, \boldsymbol{b}_3, \boldsymbol{b}_4 \in \mathbb{R}^n$ and

$$x_1 = b_1 - 2b_2 + b_3 - b_4$$

 $x_2 = -4b_1 - 2b_2 + 4b_4$
 $x_3 = 2b_1 + 3b_2 - b_3 - 3b_4$
 $x_4 = 17b_1 - 10b_2 + 11b_3 + b_4$ (2.73)

Are the vectors $x_1, \dots, x_4 \in \mathbb{R}^n$ linearly independent? To answer this question, we investigate whether the column vectors

$$\left\{ \begin{bmatrix} 1\\-2\\1\\-1 \end{bmatrix}, \begin{bmatrix} -4\\-2\\0\\4 \end{bmatrix}, \begin{bmatrix} 2\\3\\-1\\-3 \end{bmatrix}, \begin{bmatrix} 17\\-10\\11\\1 \end{bmatrix} \right\}$$
(2.74)

are linearly independent. The reduced row-echelon form of the corresponding linear equation system with coefficient matrix

$$\mathbf{A} = \begin{bmatrix} 1 & -4 & 2 & 17 \\ -2 & -2 & 3 & -10 \\ 1 & 0 & -1 & 11 \\ -1 & 4 & -3 & 1 \end{bmatrix}$$
 (2.75)

is given as

$$\begin{bmatrix} 1 & 0 & 0 & -7 \\ 0 & 1 & 0 & -15 \\ 0 & 0 & 1 & -18 \\ 0 & 0 & 0 & 0 \end{bmatrix} . (2.76)$$

We see that the corresponding linear equation system is non-trivially solvable: The last column is not a pivot column, and $x_4 = -7x_1 - 15x_2 - 18x_3$. Therefore, x_1, \ldots, x_4 are linearly dependent as x_4 can be expressed as a linear combination of x_1, \ldots, x_3 .

2.6 Basis and Rank

In a vector space V, we are particularly interested in sets of vectors \mathcal{A} that possess the property that any vector $v \in V$ can be obtained by a linear combination of vectors in \mathcal{A} . These vectors are special vectors, and in the following, we will characterize them.

2.6.1 Generating Set and Basis

Definition 2.13 (Generating Set and Span). Consider a vector space $V = (\mathcal{V}, +, \cdot)$ and set of vectors $\mathcal{A} = \{x_1, \dots, x_k\} \subseteq \mathcal{V}$. If every vector $\mathbf{v} \in \mathcal{V}$ can be expressed as a linear combination of x_1, \dots, x_k , \mathcal{A} is called a *generating set* of V. The set of all linear combinations of vectors in \mathcal{A} is called the *span* of \mathcal{A} . If \mathcal{A} spans the vector space V, we write $V = \operatorname{span}[\mathcal{A}]$ or $V = \operatorname{span}[x_1, \dots, x_k]$.

Generating sets are sets of vectors that span vector (sub)spaces, i.e., every vector can be represented as a linear combination of the vectors in the generating set. Now, we will be more specific and characterize the smallest generating set that spans a vector (sub)space.

Definition 2.14 (Basis). Consider a vector space $V = (\mathcal{V}, +, \cdot)$ and $\mathcal{A} \subseteq \mathcal{V}$. A generating set \mathcal{A} of V is called *minimal* if there exists no smaller set $\tilde{\mathcal{A}} \subseteq \mathcal{A} \subseteq \mathcal{V}$ that spans V. Every linearly independent generating set of V is minimal and is called a *basis* of V.

generating set

span

minimal

basis

Let $V=(\mathcal{V},+,\cdot)$ be a vector space and $\mathcal{B}\subseteq\mathcal{V},\mathcal{B}\neq\emptyset$. Then, the following statements are equivalent:

• \mathcal{B} is a basis of V.

• \mathcal{B} is a minimal generating set.

- \mathcal{B} is a maximal linearly independent set of vectors in V, i.e., adding any other vector to this set will make it linearly dependent.
- Every vector $x \in V$ is a linear combination of vectors from \mathcal{B} , and every linear combination is unique, i.e., with

$$\boldsymbol{x} = \sum_{i=1}^{k} \lambda_i \boldsymbol{b}_i = \sum_{i=1}^{k} \psi_i \boldsymbol{b}_i$$
 (2.77)

and $\lambda_i, \psi_i \in \mathbb{R}$, $\boldsymbol{b}_i \in \mathcal{B}$ it follows that $\lambda_i = \psi_i, i = 1, \dots, k$.

Example 2.16

• In \mathbb{R}^3 , the canonical/standard basis is

canonical basis

A basis is a minimal generating set and a

maximal linearly independent set of

vectors.

$$\mathcal{B} = \left\{ \begin{bmatrix} 1\\0\\0 \end{bmatrix}, \begin{bmatrix} 0\\1\\0 \end{bmatrix}, \begin{bmatrix} 0\\0\\1 \end{bmatrix} \right\}. \tag{2.78}$$

• Different bases in \mathbb{R}^3 are

$$\mathcal{B}_{1} = \left\{ \begin{bmatrix} 1\\0\\0 \end{bmatrix}, \begin{bmatrix} 1\\1\\0 \end{bmatrix}, \begin{bmatrix} 1\\1\\1 \end{bmatrix} \right\}, \mathcal{B}_{2} = \left\{ \begin{bmatrix} 0.5\\0.8\\0.4 \end{bmatrix}, \begin{bmatrix} 1.8\\0.3\\0.3 \end{bmatrix}, \begin{bmatrix} -2.2\\-1.3\\3.5 \end{bmatrix} \right\}. (2.79)$$

■ The set

$$\mathcal{A} = \left\{ \begin{bmatrix} 1\\2\\3\\4 \end{bmatrix}, \begin{bmatrix} 2\\-1\\0\\2 \end{bmatrix}, \begin{bmatrix} 1\\1\\0\\-4 \end{bmatrix} \right\} \tag{2.80}$$

is linearly independent, but not a generating set (and no basis) of \mathbb{R}^4 : For instance, the vector $[1,0,0,0]^\top$ cannot be obtained by a linear combination of elements in \mathcal{A} .

Remark. Every vector space V possesses a basis \mathcal{B} . The preceding examples show that there can be many bases of a vector space V, i.e., there is no unique basis. However, all bases possess the same number of elements, the *basis vectors*. \diamondsuit

basis vector

We only consider finite-dimensional vector spaces V. In this case, the dimension of V is the number of basis vectors of V, and we write $\dim(V)$. If $U \subseteq V$ is a subspace of V, then $\dim(U) \leqslant \dim(V)$ and $\dim(U) =$

dimension

 $\dim(V)$ if and only if U=V. Intuitively, the dimension of a vector space can be thought of as the number of independent directions in this vector space.

The dimension of a vector space corresponds to the number of its basis vectors.

Remark. The dimension of a vector space is not necessarily the number of elements in a vector. For instance, the vector space $V = \mathrm{span}[\begin{bmatrix} 0 \\ 1 \end{bmatrix}]$ is one-dimensional, although the basis vector possesses two elements. \diamondsuit *Remark.* A basis of a subspace $U = \mathrm{span}[\boldsymbol{x}_1, \dots, \boldsymbol{x}_m] \subseteq \mathbb{R}^n$ can be found by executing the following steps:

- 1. Write the spanning vectors as columns of a matrix A
- 2. Determine the row-echelon form of *A*.
- 3. The spanning vectors associated with the pivot columns are a basis of U.



Example 2.17 (Determining a Basis)

For a vector subspace $U \subseteq \mathbb{R}^5$, spanned by the vectors

$$m{x}_1 = egin{bmatrix} 1 \ 2 \ -1 \ -1 \ -1 \ -1 \end{bmatrix}, \quad m{x}_2 = egin{bmatrix} 2 \ -1 \ 1 \ 2 \ -2 \end{bmatrix}, \quad m{x}_3 = egin{bmatrix} 3 \ -4 \ 3 \ 5 \ -3 \end{bmatrix}, \quad m{x}_4 = egin{bmatrix} -1 \ 8 \ -5 \ -6 \ 1 \end{bmatrix} \in \mathbb{R}^5, \quad (2.81)$$

we are interested in finding out which vectors x_1, \ldots, x_4 are a basis for U. For this, we need to check whether x_1, \ldots, x_4 are linearly independent. Therefore, we need to solve

$$\sum_{i=1}^{4} \lambda_i \boldsymbol{x}_i = \boldsymbol{0} \,, \tag{2.82}$$

which leads to a homogeneous system of equations with matrix

$$[x_1, x_2, x_3, x_4] = \begin{bmatrix} 1 & 2 & 3 & -1 \\ 2 & -1 & -4 & 8 \\ -1 & 1 & 3 & -5 \\ -1 & 2 & 5 & -6 \\ -1 & -2 & -3 & 1 \end{bmatrix} .$$
 (2.83)

With the basic transformation rules for systems of linear equations, we obtain the row-echelon form

$$\begin{bmatrix} 1 & 2 & 3 & -1 \\ 2 & -1 & -4 & 8 \\ -1 & 1 & 3 & -5 \\ -1 & 2 & 5 & -6 \\ -1 & -2 & -3 & 1 \end{bmatrix} \longrightarrow \cdots \longrightarrow \begin{bmatrix} 1 & 2 & 3 & -1 \\ 0 & 1 & 2 & -2 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \end{bmatrix}.$$

Since the pivot columns indicate which set of vectors is linearly independent, we see from the row-echelon form that x_1, x_2, x_4 are linearly independent (because the system of linear equations $\lambda_1 x_1 + \lambda_2 x_2 + \lambda_4 x_4 = 0$ can only be solved with $\lambda_1 = \lambda_2 = \lambda_4 = 0$). Therefore, $\{x_1, x_2, x_4\}$ is a basis of U.

2.6.2 Rank

The number of linearly independent columns of a matrix $A \in \mathbb{R}^{m \times n}$ equals the number of linearly independent rows and is called the *rank* of A and is denoted by $\operatorname{rk}(A)$.

Remark. The rank of a matrix has some important properties:

- $\operatorname{rk}(\boldsymbol{A}) = \operatorname{rk}(\boldsymbol{A}^{\top})$, i.e., the column rank equals the row rank.
- The columns of $A \in \mathbb{R}^{m \times n}$ span a subspace $U \subseteq \mathbb{R}^m$ with $\dim(U) = \operatorname{rk}(A)$. Later we will call this subspace the *image* or *range*. A basis of U can be found by applying Gaussian elimination to A to identify the pivot columns.
- The rows of $A \in \mathbb{R}^{m \times n}$ span a subspace $W \subseteq \mathbb{R}^n$ with $\dim(W) = \operatorname{rk}(A)$. A basis of W can be found by applying Gaussian elimination to A^{\top} .
- For all $A \in \mathbb{R}^{n \times n}$ it holds that A is regular (invertible) if and only if $\operatorname{rk}(A) = n$.
- For all $A \in \mathbb{R}^{m \times n}$ and all $b \in \mathbb{R}^m$ it holds that the linear equation system Ax = b can be solved if and only if $\operatorname{rk}(A) = \operatorname{rk}(A|b)$, where A|b denotes the augmented system.
- For $A \in \mathbb{R}^{m \times n}$ the subspace of solutions for $Ax = \mathbf{0}$ possesses dimension n rk(A). Later, we will call this subspace the *kernel* or the *null space*.

kernel null space

• A matrix $A \in \mathbb{R}^{m \times n}$ has *full rank* if its rank equals the largest possible rank for a matrix of the same dimensions. This means that the rank of a full-rank matrix is the lesser of the number of rows and columns, i.e., $\operatorname{rk}(A) = \min(m,n)$. A matrix is said to be *rank deficient* if it does not have full rank.

full rank

rank deficient

\Diamond

Example 2.18 (Rank)

$$\bullet \ \mathbf{A} = \begin{bmatrix} 1 & 0 & 1 \\ 0 & 1 & 1 \\ 0 & 0 & 0 \end{bmatrix}.$$

 \boldsymbol{A} has two linearly independent rows/columns so that $rk(\boldsymbol{A}) = 2$.

We use Gaussian elimination to determine the rank:

$$\begin{bmatrix} 1 & 2 & 1 \\ -2 & -3 & 1 \\ 3 & 5 & 0 \end{bmatrix} \longrightarrow \cdots \longrightarrow \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 3 \\ 0 & 0 & 0 \end{bmatrix}. \tag{2.84}$$

Here, we see that the number of linearly independent rows and columns is 2, such that ${\rm rk}(\boldsymbol{A})=2$.

2.7 Linear Mappings

In the following, we will study mappings on vector spaces that preserve their structure, which will allow us to define the concept of a coordinate. In the beginning of the chapter, we said that vectors are objects that can be added together and multiplied by a scalar, and the resulting object is still a vector. We wish to preserve this property when applying the mapping: Consider two real vector spaces V,W. A mapping $\Phi:V\to W$ preserves the structure of the vector space if

$$\Phi(\boldsymbol{x} + \boldsymbol{y}) = \Phi(\boldsymbol{x}) + \Phi(\boldsymbol{y}) \tag{2.85}$$

$$\Phi(\lambda x) = \lambda \Phi(x) \tag{2.86}$$

for all $x, y \in V$ and $\lambda \in \mathbb{R}$. We can summarize this in the following definition:

Definition 2.15 (Linear Mapping). For vector spaces V, W, a mapping $\Phi: V \to W$ is called a *linear mapping* (or *vector space homomorphism/linear transformation*) if

$$\forall x, y \in V \,\forall \lambda, \psi \in \mathbb{R} : \Phi(\lambda x + \psi y) = \lambda \Phi(x) + \psi \Phi(y). \tag{2.87}$$

It turns out that we can represent linear mappings as matrices (Section 2.7.1). Recall that we can also collect a set of vectors as columns of a matrix. When working with matrices, we have to keep in mind what the matrix represents: a linear mapping or a collection of vectors. We will see more about linear mappings in Chapter 4. Before we continue, we will briefly introduce special mappings.

Definition 2.16 (Injective, Surjective, Bijective). Consider a mapping Φ : $\mathcal{V} \to \mathcal{W}$, where \mathcal{V}, \mathcal{W} can be arbitrary sets. Then Φ is called

- Injective if $\forall x, y \in \mathcal{V} : \Phi(x) = \Phi(y) \implies x = y$.
- Surjective if $\Phi(\mathcal{V}) = \mathcal{W}$.
- *Bijective* if it is injective and surjective.

linear mapping vector space homomorphism linear transformation

injective surjective bijective

If Φ is surjective, then every element in $\mathcal W$ can be "reached" from $\mathcal V$ using Φ . A bijective Φ can be "undone", i.e., there exists a mapping $\Psi: \mathcal W \to \mathcal V$ so that $\Psi \circ \Phi(\boldsymbol x) = \boldsymbol x$. This mapping Ψ is then called the inverse of Φ and normally denoted by Φ^{-1} .

With these definitions, we introduce the following special cases of linear mappings between vector spaces V and W:

• *Isomorphism*: $\Phi: V \to W$ linear and bijective

■ *Endomorphism*: $\Phi: V \to V$ linear

• Automorphism: $\Phi: V \to V$ linear and bijective

• We define $id_V: V \to V$, $x \mapsto x$ as the identity mapping or identity automorphism in V.

isomorphism endomorphism automorphism

identity mapping identity automorphism

Example 2.19 (Homomorphism)

The mapping $\Phi: \mathbb{R}^2 \to \mathbb{C}$, $\Phi(x) = x_1 + ix_2$, is a homomorphism:

$$\Phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix} + \begin{bmatrix} y_1 \\ y_2 \end{bmatrix}\right) = (x_1 + y_1) + i(x_2 + y_2) = x_1 + ix_2 + y_1 + iy_2$$

$$= \Phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) + \Phi\left(\begin{bmatrix} y_1 \\ y_2 \end{bmatrix}\right)$$

$$\Phi\left(\lambda \begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right) = \lambda x_1 + \lambda i x_2 = \lambda (x_1 + i x_2) = \lambda \Phi\left(\begin{bmatrix} x_1 \\ x_2 \end{bmatrix}\right).$$
(2.88)

This also justifies why complex numbers can be represented as tuples in \mathbb{R}^2 : There is a bijective linear mapping that converts the elementwise addition of tuples in \mathbb{R}^2 into the set of complex numbers with the corresponding addition. Note that we only showed linearity, but not the bijection.

Theorem 2.17 (Theorem 3.59 in Axler (2015)). *Finite-dimensional vector spaces* V *and* W *are isomorphic if and only if* $\dim(V) = \dim(W)$.

Theorem 2.17 states that there exists a linear, bijective mapping between two vector spaces of the same dimension. Intuitively, this means that vector spaces of the same dimension are kind of the same thing, as they can be transformed into each other without incurring any loss.

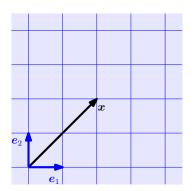
Theorem 2.17 also gives us the justification to treat $\mathbb{R}^{m\times n}$ (the vector space of $m\times n$ -matrices) and \mathbb{R}^{mn} (the vector space of vectors of length mn) the same, as their dimensions are mn, and there exists a linear, bijective mapping that transforms one into the other.

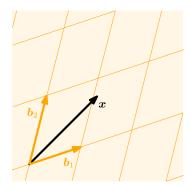
Remark. Consider vector spaces V, W, X. Then:

- For linear mappings $\Phi:V\to W$ and $\Psi:W\to X$, the mapping $\Psi\circ\Phi:V\to X$ is also linear.
- If $\Phi:V\to W$ is an isomorphism, then $\Phi^{-1}:W\to V$ is an isomorphism, too.

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Figure 2.8 Two different coordinate systems defined by two sets of basis vectors. A vector \boldsymbol{x} has different coordinate representations depending on which coordinate system is chosen.





■ If $\Phi: V \to W, \ \Psi: V \to W$ are linear, then $\Phi + \Psi$ and $\lambda \Phi, \ \lambda \in \mathbb{R}$, are linear, too.



2.7.1 Matrix Representation of Linear Mappings

Any n-dimensional vector space is isomorphic to \mathbb{R}^n (Theorem 2.17). We consider a basis $\{b_1, \ldots, b_n\}$ of an n-dimensional vector space V. In the following, the order of the basis vectors will be important. Therefore, we write

$$B = (\boldsymbol{b}_1, \dots, \boldsymbol{b}_n) \tag{2.89}$$

ordered basis

and call this n-tuple an ordered basis of V.

Remark (Notation). We are at the point where notation gets a bit tricky. Therefore, we summarize some parts here. $B=(\boldsymbol{b}_1,\ldots,\boldsymbol{b}_n)$ is an ordered basis, $\mathcal{B}=\{\boldsymbol{b}_1,\ldots,\boldsymbol{b}_n\}$ is an (unordered) basis, and $\boldsymbol{B}=[\boldsymbol{b}_1,\ldots,\boldsymbol{b}_n]$ is a matrix whose columns are the vectors $\boldsymbol{b}_1,\ldots,\boldsymbol{b}_n$.

Definition 2.18 (Coordinates). Consider a vector space V and an ordered basis $B = (\boldsymbol{b}_1, \dots, \boldsymbol{b}_n)$ of V. For any $\boldsymbol{x} \in V$ we obtain a unique representation (linear combination)

$$\boldsymbol{x} = \alpha_1 \boldsymbol{b}_1 + \ldots + \alpha_n \boldsymbol{b}_n \tag{2.90}$$

coordinate

of x with respect to B. Then $\alpha_1, \ldots, \alpha_n$ are the *coordinates* of x with respect to B, and the vector

$$\alpha = \begin{bmatrix} \alpha_1 \\ \vdots \\ \alpha_n \end{bmatrix} \in \mathbb{R}^n \tag{2.91}$$

coordinate vector coordinate representation

is the *coordinate vector/coordinate representation* of \boldsymbol{x} with respect to the ordered basis \boldsymbol{B} .

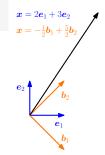
Draft (2022-01-11) of "Mathematics for Machine Learning". Feedback: https://mml-book.com.

A basis effectively defines a coordinate system. We are familiar with the Cartesian coordinate system in two dimensions, which is spanned by the canonical basis vectors $\boldsymbol{e}_1, \boldsymbol{e}_2$. In this coordinate system, a vector $\boldsymbol{x} \in \mathbb{R}^2$ has a representation that tells us how to linearly combine \boldsymbol{e}_1 and \boldsymbol{e}_2 to obtain \boldsymbol{x} . However, any basis of \mathbb{R}^2 defines a valid coordinate system, and the same vector \boldsymbol{x} from before may have a different coordinate representation in the $(\boldsymbol{b}_1, \boldsymbol{b}_2)$ basis. In Figure 2.8, the coordinates of \boldsymbol{x} with respect to the standard basis $(\boldsymbol{e}_1, \boldsymbol{e}_2)$ is $[2, 2]^{\top}$. However, with respect to the basis $(\boldsymbol{b}_1, \boldsymbol{b}_2)$ the same vector \boldsymbol{x} is represented as $[1.09, 0.72]^{\top}$, i.e., $\boldsymbol{x} = 1.09\boldsymbol{b}_1 + 0.72\boldsymbol{b}_2$. In the following sections, we will discover how to obtain this representation.

Example 2.20

Let us have a look at a geometric vector $\boldsymbol{x} \in \mathbb{R}^2$ with coordinates $[2,3]^{\top}$ with respect to the standard basis $(\boldsymbol{e}_1,\boldsymbol{e}_2)$ of \mathbb{R}^2 . This means, we can write $\boldsymbol{x}=2\boldsymbol{e}_1+3\boldsymbol{e}_2$. However, we do not have to choose the standard basis to represent this vector. If we use the basis vectors $\boldsymbol{b}_1=[1,-1]^{\top}, \boldsymbol{b}_2=[1,1]^{\top}$ we will obtain the coordinates $\frac{1}{2}[-1,5]^{\top}$ to represent the same vector with respect to $(\boldsymbol{b}_1,\boldsymbol{b}_2)$ (see Figure 2.9).

Figure 2.9 Different coordinate representations of a vector \boldsymbol{x} , depending on the choice of basis



Remark. For an n-dimensional vector space V and an ordered basis B of V, the mapping $\Phi: \mathbb{R}^n \to V$, $\Phi(e_i) = b_i$, $i = 1, \ldots, n$, is linear (and because of Theorem 2.17 an isomorphism), where (e_1, \ldots, e_n) is the standard basis of \mathbb{R}^n .

Now we are ready to make an explicit connection between matrices and linear mappings between finite-dimensional vector spaces.

Definition 2.19 (Transformation Matrix). Consider vector spaces V, W with corresponding (ordered) bases $B = (\boldsymbol{b}_1, \dots, \boldsymbol{b}_n)$ and $C = (\boldsymbol{c}_1, \dots, \boldsymbol{c}_m)$. Moreover, we consider a linear mapping $\Phi : V \to W$. For $j \in \{1, \dots, n\}$,

$$\Phi(\boldsymbol{b}_j) = \alpha_{1j}\boldsymbol{c}_1 + \dots + \alpha_{mj}\boldsymbol{c}_m = \sum_{i=1}^m \alpha_{ij}\boldsymbol{c}_i$$
 (2.92)

is the unique representation of $\Phi(b_j)$ with respect to C. Then, we call the $m \times n$ -matrix A_{Φ} , whose elements are given by

$$A_{\Phi}(i,j) = \alpha_{ij} \,, \tag{2.93}$$

the transformation matrix of Φ (with respect to the ordered bases B of V and C of W).

transformation matrix

The coordinates of $\Phi(b_j)$ with respect to the ordered basis C of W are the j-th column of A_{Φ} . Consider (finite-dimensional) vector spaces V, W with ordered bases B, C and a linear mapping $\Phi: V \to W$ with

transformation matrix A_{Φ} . If \hat{x} is the coordinate vector of $x \in V$ with respect to B and \hat{y} the coordinate vector of $y = \Phi(x) \in W$ with respect to C, then

$$\hat{y} = A_{\Phi} \hat{x} \,. \tag{2.94}$$

This means that the transformation matrix can be used to map coordinates with respect to an ordered basis in V to coordinates with respect to an ordered basis in W.

Example 2.21 (Transformation Matrix)

Consider a homomorphism $\Phi:V\to W$ and ordered bases $B=(\boldsymbol{b}_1,\ldots,\boldsymbol{b}_3)$ of V and $C=(\boldsymbol{c}_1,\ldots,\boldsymbol{c}_4)$ of W. With

$$\Phi(\mathbf{b}_1) = \mathbf{c}_1 - \mathbf{c}_2 + 3\mathbf{c}_3 - \mathbf{c}_4
\Phi(\mathbf{b}_2) = 2\mathbf{c}_1 + \mathbf{c}_2 + 7\mathbf{c}_3 + 2\mathbf{c}_4
\Phi(\mathbf{b}_3) = 3\mathbf{c}_2 + \mathbf{c}_3 + 4\mathbf{c}_4$$
(2.95)

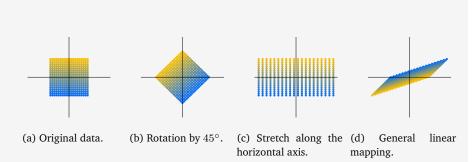
the transformation matrix A_{Φ} with respect to B and C satisfies $\Phi(b_k) = \sum_{i=1}^4 \alpha_{ik} c_i$ for $k = 1, \dots, 3$ and is given as

$$A_{\Phi} = [\alpha_1, \alpha_2, \alpha_3] = \begin{bmatrix} 1 & 2 & 0 \\ -1 & 1 & 3 \\ 3 & 7 & 1 \\ -1 & 2 & 4 \end{bmatrix},$$
 (2.96)

where the $\alpha_j,\ j=1,2,3,$ are the coordinate vectors of $\Phi(\boldsymbol{b}_j)$ with respect to C.

Example 2.22 (Linear Transformations of Vectors)

Figure 2.10 Three examples of linear transformations of the vectors shown as dots in (a); (b) Rotation by 45°; (c) Stretching of the horizontal coordinates by 2; (d) Combination of reflection, rotation and stretching.



We consider three linear transformations of a set of vectors in \mathbb{R}^2 with the transformation matrices

$$\boldsymbol{A}_{1} = \begin{bmatrix} \cos(\frac{\pi}{4}) & -\sin(\frac{\pi}{4}) \\ \sin(\frac{\pi}{4}) & \cos(\frac{\pi}{4}) \end{bmatrix}, \ \boldsymbol{A}_{2} = \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix}, \ \boldsymbol{A}_{3} = \frac{1}{2} \begin{bmatrix} 3 & -1 \\ 1 & -1 \end{bmatrix}.$$
 (2.97)

Figure 2.10 gives three examples of linear transformations of a set of vectors. Figure 2.10(a) shows 400 vectors in \mathbb{R}^2 , each of which is represented by a dot at the corresponding (x_1,x_2) -coordinates. The vectors are arranged in a square. When we use matrix A_1 in (2.97) to linearly transform each of these vectors, we obtain the rotated square in Figure 2.10(b). If we apply the linear mapping represented by A_2 , we obtain the rectangle in Figure 2.10(c) where each x_1 -coordinate is stretched by 2. Figure 2.10(d) shows the original square from Figure 2.10(a) when linearly transformed using A_3 , which is a combination of a reflection, a rotation, and a stretch.

2.7.2 Basis Change

In the following, we will have a closer look at how transformation matrices of a linear mapping $\Phi:V\to W$ change if we change the bases in V and W. Consider two ordered bases

$$B = (\boldsymbol{b}_1, \dots, \boldsymbol{b}_n), \quad \tilde{B} = (\tilde{\boldsymbol{b}}_1, \dots, \tilde{\boldsymbol{b}}_n)$$
 (2.98)

of V and two ordered bases

$$C = (\boldsymbol{c}_1, \dots, \boldsymbol{c}_m), \quad \tilde{C} = (\tilde{\boldsymbol{c}}_1, \dots, \tilde{\boldsymbol{c}}_m)$$
 (2.99)

of W. Moreover, $\mathbf{A}_{\Phi} \in \mathbb{R}^{m \times n}$ is the transformation matrix of the linear mapping $\Phi: V \to W$ with respect to the bases B and C, and $\tilde{\mathbf{A}}_{\Phi} \in \mathbb{R}^{m \times n}$ is the corresponding transformation mapping with respect to \tilde{B} and \tilde{C} . In the following, we will investigate how \mathbf{A} and $\tilde{\mathbf{A}}$ are related, i.e., how/whether we can transform \mathbf{A}_{Φ} into $\tilde{\mathbf{A}}_{\Phi}$ if we choose to perform a basis change from B, C to \tilde{B}, \tilde{C} .

Remark. We effectively get different coordinate representations of the identity mapping id_V . In the context of Figure 2.9, this would mean to map coordinates with respect to (e_1,e_2) onto coordinates with respect to (b_1,b_2) without changing the vector x. By changing the basis and correspondingly the representation of vectors, the transformation matrix with respect to this new basis can have a particularly simple form that allows for straightforward computation.

Example 2.23 (Basis Change)

Consider a transformation matrix

$$\boldsymbol{A} = \begin{bmatrix} 2 & 1 \\ 1 & 2 \end{bmatrix} \tag{2.100}$$

with respect to the canonical basis in \mathbb{R}^2 . If we define a new basis

$$B = \begin{pmatrix} 1\\1 \end{pmatrix}, \begin{bmatrix} 1\\-1 \end{bmatrix}$$
 (2.101)

we obtain a diagonal transformation matrix

$$\tilde{\boldsymbol{A}} = \begin{bmatrix} 3 & 0 \\ 0 & 1 \end{bmatrix} \tag{2.102}$$

with respect to B, which is easier to work with than A.

In the following, we will look at mappings that transform coordinate vectors with respect to one basis into coordinate vectors with respect to a different basis. We will state our main result first and then provide an explanation.

Theorem 2.20 (Basis Change). For a linear mapping $\Phi: V \to W$, ordered bases

$$B = (\boldsymbol{b}_1, \dots, \boldsymbol{b}_n), \quad \tilde{B} = (\tilde{\boldsymbol{b}}_1, \dots, \tilde{\boldsymbol{b}}_n) \tag{2.103}$$

of V and

$$C = (\boldsymbol{c}_1, \dots, \boldsymbol{c}_m), \quad \tilde{C} = (\tilde{\boldsymbol{c}}_1, \dots, \tilde{\boldsymbol{c}}_m)$$
 (2.104)

of W, and a transformation matrix \mathbf{A}_{Φ} of Φ with respect to B and C, the corresponding transformation matrix $\tilde{\mathbf{A}}_{\Phi}$ with respect to the bases \tilde{B} and \tilde{C} is given as

$$\tilde{\boldsymbol{A}}_{\Phi} = \boldsymbol{T}^{-1} \boldsymbol{A}_{\Phi} \boldsymbol{S} \,. \tag{2.105}$$

Here, $S \in \mathbb{R}^{n \times n}$ is the transformation matrix of id_V that maps coordinates with respect to \tilde{B} onto coordinates with respect to B, and $T \in \mathbb{R}^{m \times m}$ is the transformation matrix of id_W that maps coordinates with respect to \tilde{C} onto coordinates with respect to C.

Proof Following Drumm and Weil (2001), we can write the vectors of the new basis \tilde{B} of V as a linear combination of the basis vectors of B, such that

$$\tilde{\boldsymbol{b}}_{j} = s_{1j}\boldsymbol{b}_{1} + \dots + s_{nj}\boldsymbol{b}_{n} = \sum_{i=1}^{n} s_{ij}\boldsymbol{b}_{i}, \quad j = 1,\dots,n.$$
 (2.106)

Similarly, we write the new basis vectors \tilde{C} of W as a linear combination of the basis vectors of C, which yields

$$\tilde{\boldsymbol{c}}_k = t_{1k} \boldsymbol{c}_1 + \dots + t_{mk} \boldsymbol{c}_m = \sum_{l=1}^m t_{lk} \boldsymbol{c}_l, \quad k = 1, \dots, m.$$
 (2.107)

We define $S = ((s_{ij})) \in \mathbb{R}^{n \times n}$ as the transformation matrix that maps coordinates with respect to \tilde{B} onto coordinates with respect to B and $T = ((t_{lk})) \in \mathbb{R}^{m \times m}$ as the transformation matrix that maps coordinates with respect to \tilde{C} onto coordinates with respect to C. In particular, the jth column of S is the coordinate representation of \tilde{b}_j with respect to B and

the kth column of T is the coordinate representation of \tilde{c}_k with respect to C. Note that both S and T are regular.

We are going to look at $\Phi(\hat{b}_j)$ from two perspectives. First, applying the mapping Φ , we get that for all j = 1, ..., n

$$\Phi(\tilde{\boldsymbol{b}}_{j}) = \sum_{k=1}^{m} \tilde{a}_{kj} \tilde{\boldsymbol{c}}_{k} \stackrel{(2.107)}{=} \sum_{k=1}^{m} \tilde{a}_{kj} \sum_{l=1}^{m} t_{lk} \boldsymbol{c}_{l} = \sum_{l=1}^{m} \left(\sum_{k=1}^{m} t_{lk} \tilde{a}_{kj} \right) \boldsymbol{c}_{l}, \quad (2.108)$$

where we first expressed the new basis vectors $\tilde{\boldsymbol{c}}_k \in W$ as linear combinations of the basis vectors $\boldsymbol{c}_l \in W$ and then swapped the order of summation

Alternatively, when we express the $\tilde{\boldsymbol{b}}_j \in V$ as linear combinations of $\boldsymbol{b}_j \in V$, we arrive at

$$\Phi(\tilde{\boldsymbol{b}}_{j}) \stackrel{(2.106)}{=} \Phi\left(\sum_{i=1}^{n} s_{ij} \boldsymbol{b}_{i}\right) = \sum_{i=1}^{n} s_{ij} \Phi(\boldsymbol{b}_{i}) = \sum_{i=1}^{n} s_{ij} \sum_{l=1}^{m} a_{li} \boldsymbol{c}_{l} \quad (2.109a)$$

$$= \sum_{l=1}^{m} \left(\sum_{i=1}^{n} a_{li} s_{ij}\right) \boldsymbol{c}_{l}, \quad j = 1, \dots, n, \quad (2.109b)$$

it follows for all j = 1, ..., n and l = 1, ..., m that

 $= \sum_{l=1} \left(\sum_{i=1} a_{li} s_{ij}\right) c_l, \quad j = 1, \dots, n,$ (2.109b)
where we exploited the linearity of Φ . Comparing (2.108) and (2.109b),

$$\sum_{l}^{m} t_{lk} \tilde{a}_{kj} = \sum_{l}^{n} a_{li} s_{ij} \tag{2.110}$$

and, therefore,

$$T\tilde{A}_{\Phi} = A_{\Phi}S \in \mathbb{R}^{m \times n}$$
, (2.111)

such that

$$\tilde{\boldsymbol{A}}_{\Phi} = \boldsymbol{T}^{-1} \boldsymbol{A}_{\Phi} \boldsymbol{S} \,, \tag{2.112}$$

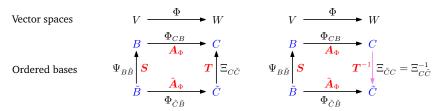
which proves Theorem 2.20.

Theorem 2.20 tells us that with a basis change in V (B is replaced with \tilde{B}) and W (C is replaced with \tilde{C}), the transformation matrix A_{Φ} of a linear mapping $\Phi: V \to W$ is replaced by an equivalent matrix \tilde{A}_{Φ} with

$$\tilde{\boldsymbol{A}}_{\Phi} = \boldsymbol{T}^{-1} \boldsymbol{A}_{\Phi} \boldsymbol{S}. \tag{2.113}$$

Figure 2.11 illustrates this relation: Consider a homomorphism $\Phi:V\to W$ and ordered bases B,\tilde{B} of V and C,\tilde{C} of W. The mapping Φ_{CB} is an instantiation of Φ and maps basis vectors of B onto linear combinations of basis vectors of C. Assume that we know the transformation matrix \mathbf{A}_{Φ} of Φ_{CB} with respect to the ordered bases B,C. When we perform a basis change from B to \tilde{B} in V and from C to \tilde{C} in W, we can determine the

Figure 2.11 For a homomorphism $\Phi:V\to W$ and ordered bases B, \tilde{B} of V and C, \tilde{C} of W (marked in blue), we can express the mapping $\Phi_{\tilde{C}\tilde{B}}$ with respect to the bases \tilde{B}, \tilde{C} equivalently as a composition of the homomorphisms $\Phi_{\tilde{C}\tilde{B}} =$ $\Xi_{\tilde{C}C} \circ \Phi_{CB} \circ \Psi_{B\tilde{B}}$ with respect to the bases in the subscripts. The corresponding transformation matrices are in red.



corresponding transformation matrix \tilde{A}_{Φ} as follows: First, we find the matrix representation of the linear mapping $\Psi_{B\tilde{B}}:V\to V$ that maps coordinates with respect to the new basis \tilde{B} onto the (unique) coordinates with respect to the "old" basis B (in V). Then, we use the transformation matrix A_{Φ} of $\Phi_{CB}:V\to W$ to map these coordinates onto the coordinates with respect to C in W. Finally, we use a linear mapping $\Xi_{\tilde{C}C}:W\to W$ to map the coordinates with respect to C onto coordinates with respect to C. Therefore, we can express the linear mapping $\Phi_{\tilde{C}\tilde{B}}$ as a composition of linear mappings that involve the "old" basis:

$$\Phi_{\tilde{C}\tilde{B}} = \Xi_{\tilde{C}C} \circ \Phi_{CB} \circ \Psi_{B\tilde{B}} = \Xi_{C\tilde{C}}^{-1} \circ \Phi_{CB} \circ \Psi_{B\tilde{B}}. \tag{2.114}$$

Concretely, we use $\Psi_{B\tilde{B}}=\mathrm{id}_V$ and $\Xi_{C\tilde{C}}=\mathrm{id}_W$, i.e., the identity mappings that map vectors onto themselves, but with respect to a different basis.

equivalent

similar

Definition 2.21 (Equivalence). Two matrices $A, A \in \mathbb{R}^{m \times n}$ are equivalent if there exist regular matrices $S \in \mathbb{R}^{n \times n}$ and $T \in \mathbb{R}^{m \times m}$, such that $\tilde{A} = T^{-1}AS$.

Definition 2.22 (Similarity). Two matrices $A, \tilde{A} \in \mathbb{R}^{n \times n}$ are *similar* if there exists a regular matrix $S \in \mathbb{R}^{n \times n}$ with $\tilde{A} = S^{-1}AS$

Remark. Similar matrices are always equivalent. However, equivalent matrices are not necessarily similar. \Diamond

Remark. Consider vector spaces V,W,X. From the remark that follows Theorem 2.17, we already know that for linear mappings $\Phi:V\to W$ and $\Psi:W\to X$ the mapping $\Psi\circ\Phi:V\to X$ is also linear. With transformation matrices ${\bf A}_\Phi$ and ${\bf A}_\Psi$ of the corresponding mappings, the overall transformation matrix is ${\bf A}_{\Psi\circ\Phi}={\bf A}_\Psi{\bf A}_\Phi$.

In light of this remark, we can look at basis changes from the perspective of composing linear mappings:

- A_{Φ} is the transformation matrix of a linear mapping $\Phi_{CB}:V\to W$ with respect to the bases B,C.
- \tilde{A}_{Φ} is the transformation matrix of the linear mapping $\Phi_{\tilde{C}\tilde{B}}:V\to W$ with respect to the bases \tilde{B},\tilde{C} .
- S is the transformation matrix of a linear mapping $\Psi_{B\tilde{B}}:V\to V$ (automorphism) that represents \tilde{B} in terms of B. Normally, $\Psi=\mathrm{id}_V$ is the identity mapping in V.

■ T is the transformation matrix of a linear mapping $\Xi_{C\tilde{C}}: W \to W$ (automorphism) that represents \tilde{C} in terms of C. Normally, $\Xi = \mathrm{id}_W$ is the identity mapping in W.

If we (informally) write down the transformations just in terms of bases, then $A_{\Phi}: B \to C$, $\tilde{A}_{\Phi}: \tilde{B} \to \tilde{C}$, $S: \tilde{B} \to B$, $T: \tilde{C} \to C$ and $T^{-1}: C \to \tilde{C}$, and

$$\tilde{B} \to \tilde{C} = \tilde{B} \to B \to C \to \tilde{C}$$
 (2.115)

$$\tilde{\boldsymbol{A}}_{\Phi} = \boldsymbol{T}^{-1} \boldsymbol{A}_{\Phi} \boldsymbol{S} \,. \tag{2.116}$$

Note that the execution order in (2.116) is from right to left because vectors are multiplied at the right-hand side so that $x\mapsto Sx\mapsto A_\Phi(Sx)\mapsto T^{-1}\big(A_\Phi(Sx)\big)=\tilde{A}_\Phi x.$

Example 2.24 (Basis Change)

Consider a linear mapping $\Phi: \mathbb{R}^3 \to \mathbb{R}^4$ whose transformation matrix is

$$\boldsymbol{A}_{\Phi} = \begin{bmatrix} 1 & 2 & 0 \\ -1 & 1 & 3 \\ 3 & 7 & 1 \\ -1 & 2 & 4 \end{bmatrix}$$
 (2.117)

with respect to the standard bases

$$B = \begin{pmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \end{bmatrix} \end{pmatrix}, \quad C = \begin{pmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \end{pmatrix}. \tag{2.118}$$

We seek the transformation matrix $\tilde{\boldsymbol{A}}_{\Phi}$ of Φ with respect to the new bases

$$\tilde{B} = (\begin{bmatrix} 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \end{bmatrix}) \in \mathbb{R}^3, \quad \tilde{C} = (\begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 0 \\ 1 \\ 1 \\ 0 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}). \quad (2.119)$$

Then,

$$S = \begin{bmatrix} 1 & 0 & 1 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{bmatrix}, \qquad T = \begin{bmatrix} 1 & 1 & 0 & 1 \\ 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, \tag{2.120}$$

where the *i*th column of S is the coordinate representation of $\tilde{\boldsymbol{b}}_i$ in terms of the basis vectors of B. Since B is the standard basis, the coordinate representation is straightforward to find. For a general basis B, we would need to solve a linear equation system to find the λ_i such that

 $\sum_{i=1}^{3} \lambda_i b_i = \tilde{b}_j$, $j = 1, \dots, 3$. Similarly, the jth column of T is the coordinate representation of \tilde{c}_i in terms of the basis vectors of C.

Therefore, we obtain

$$\tilde{\boldsymbol{A}}_{\Phi} = \boldsymbol{T}^{-1} \boldsymbol{A}_{\Phi} \boldsymbol{S} = \frac{1}{2} \begin{bmatrix} 1 & 1 & -1 & -1 \\ 1 & -1 & 1 & -1 \\ -1 & 1 & 1 & 1 \\ 0 & 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} 3 & 2 & 1 \\ 0 & 4 & 2 \\ 10 & 8 & 4 \\ 1 & 6 & 3 \end{bmatrix}$$
(2.121a)

$$= \begin{bmatrix} -4 & -4 & -2 \\ 6 & 0 & 0 \\ 4 & 8 & 4 \\ 1 & 6 & 3 \end{bmatrix}. \tag{2.121b}$$

In Chapter 4, we will be able to exploit the concept of a basis change to find a basis with respect to which the transformation matrix of an endomorphism has a particularly simple (diagonal) form. In Chapter 10, we will look at a data compression problem and find a convenient basis onto which we can project the data while minimizing the compression loss.

2.7.3 Image and Kernel

The image and kernel of a linear mapping are vector subspaces with certain important properties. In the following, we will characterize them more carefully.

Definition 2.23 (Image and Kernel).

For $\Phi: V \to W$, we define the *kernel/null space*

$$\ker(\Phi) := \Phi^{-1}(\mathbf{0}_W) = \{ v \in V : \Phi(v) = \mathbf{0}_W \}$$
 (2.122)

and the image/range

$$\operatorname{Im}(\Phi) := \Phi(V) = \{ w \in W | \exists v \in V : \Phi(v) = w \}.$$
 (2.123)

We also call V and W the domain and codomain of Φ , respectively.

Intuitively, the kernel is the set of vectors $v \in V$ that Φ maps onto the neutral element $\mathbf{0}_W \in W$. The image is the set of vectors $w \in W$ that can be "reached" by Φ from any vector in V. An illustration is given in Figure 2.12.

Remark. Consider a linear mapping $\Phi:V\to W,$ where $V\!,W$ are vector spaces.

- It always holds that $\Phi(\mathbf{0}_V) = \mathbf{0}_W$ and, therefore, $\mathbf{0}_V \in \ker(\Phi)$. In particular, the null space is never empty.
- $\operatorname{Im}(\Phi) \subseteq W$ is a subspace of W, and $\ker(\Phi) \subseteq V$ is a subspace of V.

kernel null space

image range

domain codomain

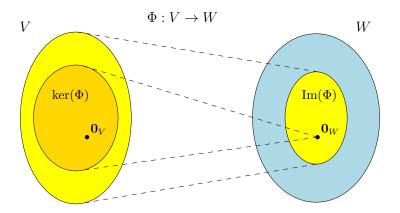


Figure 2.12 Kernel and image of a linear mapping $\Phi: V \to W$.

• Φ is injective (one-to-one) if and only if $\ker(\Phi) = \{0\}$.

Δ

Remark (Null Space and Column Space). Let us consider $A \in \mathbb{R}^{m \times n}$ and a linear mapping $\Phi : \mathbb{R}^n \to \mathbb{R}^m$, $x \mapsto Ax$.

• For $A = [a_1, \dots, a_n]$, where a_i are the columns of A, we obtain

$$\operatorname{Im}(\Phi) = \left\{ \mathbf{A} \mathbf{x} : \mathbf{x} \in \mathbb{R}^n \right\} = \left\{ \sum_{i=1}^n x_i \mathbf{a}_i : x_1, \dots, x_n \in \mathbb{R} \right\} \quad (2.124a)$$
$$= \operatorname{span}[\mathbf{a}_1, \dots, \mathbf{a}_n] \subseteq \mathbb{R}^m, \quad (2.124b)$$

i.e., the image is the span of the columns of A, also called the *column space*. Therefore, the column space (image) is a subspace of \mathbb{R}^m , where m is the "height" of the matrix.

column space

- $\operatorname{rk}(\boldsymbol{A}) = \dim(\operatorname{Im}(\Phi)).$
- The kernel/null space $\ker(\Phi)$ is the general solution to the homogeneous system of linear equations $Ax = \mathbf{0}$ and captures all possible linear combinations of the elements in \mathbb{R}^n that produce $\mathbf{0} \in \mathbb{R}^m$.
- The kernel is a subspace of \mathbb{R}^n , where n is the "width" of the matrix.
- The kernel focuses on the relationship among the columns, and we can use it to determine whether/how we can express a column as a linear combination of other columns.



Example 2.25 (Image and Kernel of a Linear Mapping) The mapping

$$\Phi: \mathbb{R}^4 \to \mathbb{R}^2, \quad \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} \mapsto \begin{bmatrix} 1 & 2 & -1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} x_1 + 2x_2 - x_3 \\ x_1 + x_4 \end{bmatrix}$$
(2.125a)

$$=x_1\begin{bmatrix}1\\1\end{bmatrix}+x_2\begin{bmatrix}2\\0\end{bmatrix}+x_3\begin{bmatrix}-1\\0\end{bmatrix}+x_4\begin{bmatrix}0\\1\end{bmatrix} \quad \text{(2.125b)}$$

is linear. To determine $\mathrm{Im}(\Phi)$, we can take the span of the columns of the transformation matrix and obtain

$$\operatorname{Im}(\Phi) = \operatorname{span}\begin{bmatrix} 1\\1 \end{bmatrix}, \begin{bmatrix} 2\\0 \end{bmatrix}, \begin{bmatrix} -1\\0 \end{bmatrix}, \begin{bmatrix} 0\\1 \end{bmatrix}]. \tag{2.126}$$

To compute the kernel (null space) of Φ , we need to solve Ax = 0, i.e., we need to solve a homogeneous equation system. To do this, we use Gaussian elimination to transform A into reduced row-echelon form:

$$\begin{bmatrix} 1 & 2 & -1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \longrightarrow \cdots \longrightarrow \begin{bmatrix} 1 & 0 & 0 & 1 \\ 0 & 1 & -\frac{1}{2} & -\frac{1}{2} \end{bmatrix}. \tag{2.127}$$

This matrix is in reduced row-echelon form, and we can use the Minus-1 Trick to compute a basis of the kernel (see Section 2.3.3). Alternatively, we can express the non-pivot columns (columns 3 and 4) as linear combinations of the pivot columns (columns 1 and 2). The third column a_3 is equivalent to $-\frac{1}{2}$ times the second column a_2 . Therefore, $0 = a_3 + \frac{1}{2}a_2$. In the same way, we see that $a_4 = a_1 - \frac{1}{2}a_2$ and, therefore, $0 = a_1 - \frac{1}{2}a_2 - a_4$. Overall, this gives us the kernel (null space) as

$$\ker(\Phi) = \operatorname{span}\begin{bmatrix} 0\\ \frac{1}{2}\\ 1\\ 0 \end{bmatrix}, \begin{bmatrix} -1\\ \frac{1}{2}\\ 0\\ 1 \end{bmatrix}. \tag{2.128}$$

rank-nullity theorem

Theorem 2.24 (Rank-Nullity Theorem). For vector spaces V, W and a linear mapping $\Phi: V \to W$ it holds that

$$\dim(\ker(\Phi)) + \dim(\operatorname{Im}(\Phi)) = \dim(V). \tag{2.129}$$

fundamental theorem of linear mappings The rank-nullity theorem is also referred to as the *fundamental theorem* of *linear mappings* (Axler, 2015, theorem 3.22). The following are direct consequences of Theorem 2.24:

- If $\dim(\operatorname{Im}(\Phi)) < \dim(V)$, then $\ker(\Phi)$ is non-trivial, i.e., the kernel contains more than $\mathbf{0}_V$ and $\dim(\ker(\Phi)) \geqslant 1$.
- If A_{Φ} is the transformation matrix of Φ with respect to an ordered basis and $\dim(\operatorname{Im}(\Phi)) < \dim(V)$, then the system of linear equations $A_{\Phi}x = \mathbf{0}$ has infinitely many solutions.
- If $\dim(V) = \dim(W)$, then the following three-way equivalence holds:
 - Φ is injective
 - Φ is surjective
 - Φ is bijective

since $\operatorname{Im}(\Phi) \subseteq W$.

2.8 Affine Spaces

In the following, we will have a closer look at spaces that are offset from the origin, i.e., spaces that are no longer vector subspaces. Moreover, we will briefly discuss properties of mappings between these affine spaces, which resemble linear mappings.

Remark. In the machine learning literature, the distinction between linear and affine is sometimes not clear so that we can find references to affine spaces/mappings as linear spaces/mappings. ♢

2.8.1 Affine Subspaces

Definition 2.25 (Affine Subspace). Let V be a vector space, $x_0 \in V$ and $U \subseteq V$ a subspace. Then the subset

$$L = x_0 + U := \{x_0 + u : u \in U\}$$
 (2.130a)

$$= \{ \boldsymbol{v} \in V | \exists \boldsymbol{u} \in U : \boldsymbol{v} = \boldsymbol{x}_0 + \boldsymbol{u} \} \subseteq V$$
 (2.130b)

is called affine subspace or linear manifold of V. U is called direction or direction space, and \boldsymbol{x}_0 is called support point. In Chapter 12, we refer to such a subspace as a hyperplane.

affine subspace linear manifold direction direction space support point hyperplane

Note that the definition of an affine subspace excludes $\mathbf{0}$ if $\mathbf{x}_0 \notin U$. Therefore, an affine subspace is not a (linear) subspace (vector subspace) of V for $\mathbf{x}_0 \notin U$.

Examples of affine subspaces are points, lines, and planes in \mathbb{R}^3 , which do not (necessarily) go through the origin.

Remark. Consider two affine subspaces $L = \boldsymbol{x}_0 + U$ and $\tilde{L} = \tilde{\boldsymbol{x}}_0 + \tilde{U}$ of a vector space V. Then, $L \subseteq \tilde{L}$ if and only if $U \subseteq \tilde{U}$ and $\boldsymbol{x}_0 - \tilde{\boldsymbol{x}}_0 \in \tilde{U}$.

Affine subspaces are often described by *parameters*: Consider a k-dimensional affine space $L = x_0 + U$ of V. If (b_1, \ldots, b_k) is an ordered basis of U, then every element $x \in L$ can be uniquely described as

$$x = x_0 + \lambda_1 b_1 + \ldots + \lambda_k b_k, \qquad (2.131)$$

where $\lambda_1, \ldots, \lambda_k \in \mathbb{R}$. This representation is called *parametric equation* of L with directional vectors $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_k$ and *parameters* $\lambda_1, \ldots, \lambda_k$.

parametric equation parameters

Example 2.26 (Affine Subspaces)

• One-dimensional affine subspaces are called *lines* and can be written as $\boldsymbol{y} = \boldsymbol{x}_0 + \lambda \boldsymbol{b}_1$, where $\lambda \in \mathbb{R}$ and $U = \operatorname{span}[\boldsymbol{b}_1] \subseteq \mathbb{R}^n$ is a one-dimensional subspace of \mathbb{R}^n . This means that a line is defined by a support point \boldsymbol{x}_0 and a vector \boldsymbol{b}_1 that defines the direction. See Figure 2.13 for an illustration.

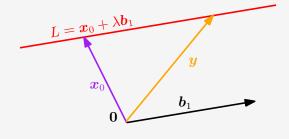
plane

hyperplane

Figure 2.13 Lines are affine subspaces. Vectors y on a line $x_0 + \lambda b_1$ lie in an affine subspace L with support point x_0 and direction b_1 .

■ Two-dimensional affine subspaces of \mathbb{R}^n are called *planes*. The parametric equation for planes is $\mathbf{y} = \mathbf{x}_0 + \lambda_1 \mathbf{b}_1 + \lambda_2 \mathbf{b}_2$, where $\lambda_1, \lambda_2 \in \mathbb{R}$ and $U = \operatorname{span}[\mathbf{b}_1, \mathbf{b}_2] \subseteq \mathbb{R}^n$. This means that a plane is defined by a support point \mathbf{x}_0 and two linearly independent vectors $\mathbf{b}_1, \mathbf{b}_2$ that span the direction space.

■ In \mathbb{R}^n , the (n-1)-dimensional affine subspaces are called *hyperplanes*, and the corresponding parametric equation is $\boldsymbol{y} = \boldsymbol{x}_0 + \sum_{i=1}^{n-1} \lambda_i \boldsymbol{b}_i$, where $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_{n-1}$ form a basis of an (n-1)-dimensional subspace U of \mathbb{R}^n . This means that a hyperplane is defined by a support point \boldsymbol{x}_0 and (n-1) linearly independent vectors $\boldsymbol{b}_1, \ldots, \boldsymbol{b}_{n-1}$ that span the direction space. In \mathbb{R}^2 , a line is also a hyperplane. In \mathbb{R}^3 , a plane is also a hyperplane.



Remark (Inhomogeneous systems of linear equations and affine subspaces). For $A \in \mathbb{R}^{m \times n}$ and $x \in \mathbb{R}^m$, the solution of the system of linear equations $A\lambda = x$ is either the empty set or an affine subspace of \mathbb{R}^n of dimension n - rk(A). In particular, the solution of the linear equation $\lambda_1 b_1 + \ldots + \lambda_n b_n = x$, where $(\lambda_1, \ldots, \lambda_n) \neq (0, \ldots, 0)$, is a hyperplane in \mathbb{R}^n .

In \mathbb{R}^n , every k-dimensional affine subspace is the solution of an inhomogeneous system of linear equations Ax = b, where $A \in \mathbb{R}^{m \times n}$, $b \in \mathbb{R}^m$ and $\mathrm{rk}(A) = n - k$. Recall that for homogeneous equation systems Ax = 0 the solution was a vector subspace, which we can also think of as a special affine space with support point $x_0 = 0$.

2.8.2 Affine Mappings

Similar to linear mappings between vector spaces, which we discussed in Section 2.7, we can define affine mappings between two affine spaces. Linear and affine mappings are closely related. Therefore, many properties that we already know from linear mappings, e.g., that the composition of linear mappings is a linear mapping, also hold for affine mappings.

Definition 2.26 (Affine Mapping). For two vector spaces V, W, a linear

mapping $\Phi: V \to W$, and $a \in W$, the mapping

$$\phi: V \to W \tag{2.132}$$

$$\boldsymbol{x} \mapsto \boldsymbol{a} + \Phi(\boldsymbol{x}) \tag{2.133}$$

is an affine mapping from V to W. The vector \boldsymbol{a} is called the translation vector of ϕ .

affine mapping translation vector

- Every affine mapping $\phi: V \to W$ is also the composition of a linear mapping $\Phi: V \to W$ and a translation $\tau: W \to W$ in W, such that $\phi = \tau \circ \Phi$. The mappings Φ and τ are uniquely determined.
- The composition $\phi' \circ \phi$ of affine mappings $\phi: V \to W$, $\phi': W \to X$ is affine.
- Affine mappings keep the geometric structure invariant. They also preserve the dimension and parallelism.

2.9 Further Reading

There are many resources for learning linear algebra, including the text-books by Strang (2003), Golan (2007), Axler (2015), and Liesen and Mehrmann (2015). There are also several online resources that we mentioned in the introduction to this chapter. We only covered Gaussian elimination here, but there are many other approaches for solving systems of linear equations, and we refer to numerical linear algebra textbooks by Stoer and Burlirsch (2002), Golub and Van Loan (2012), and Horn and Johnson (2013) for an in-depth discussion.

In this book, we distinguish between the topics of linear algebra (e.g., vectors, matrices, linear independence, basis) and topics related to the geometry of a vector space. In Chapter 3, we will introduce the inner product, which induces a norm. These concepts allow us to define angles, lengths and distances, which we will use for orthogonal projections. Projections turn out to be key in many machine learning algorithms, such as linear regression and principal component analysis, both of which we will cover in Chapters 9 and 10, respectively.

Exercises

2.1 We consider $(\mathbb{R}\setminus\{-1\},\star)$, where

$$a \star b := ab + a + b, \qquad a, b \in \mathbb{R} \setminus \{-1\}$$
 (2.134)

- a. Show that $(\mathbb{R}\setminus\{-1\},\star)$ is an Abelian group.
- b. Solve

$$3 \star x \star x = 15$$

in the Abelian group $(\mathbb{R}\setminus\{-1\},\star)$, where \star is defined in (2.134).

2.2 Let n be in $\mathbb{N}\setminus\{0\}$. Let k, x be in \mathbb{Z} . We define the congruence class \bar{k} of the integer k as the set

$$\overline{k} = \{ x \in \mathbb{Z} \mid x - k = 0 \pmod{n} \}$$
$$= \{ x \in \mathbb{Z} \mid \exists a \in \mathbb{Z} \colon (x - k = n \cdot a) \}.$$

We now define $\mathbb{Z}/n\mathbb{Z}$ (sometimes written \mathbb{Z}_n) as the set of all congruence classes modulo n. Euclidean division implies that this set is a finite set containing n elements:

$$\mathbb{Z}_n = \{\overline{0}, \overline{1}, \dots, \overline{n-1}\}$$

For all $\overline{a}, \overline{b} \in \mathbb{Z}_n$, we define

$$\overline{a}\oplus \overline{b}:=\overline{a+b}$$

- a. Show that (\mathbb{Z}_n, \oplus) is a group. Is it Abelian?
- b. We now define another operation \otimes for all \bar{a} and \bar{b} in \mathbb{Z}_n as

$$\overline{a} \otimes \overline{b} = \overline{a \times b}, \qquad (2.135)$$

where $a \times b$ represents the usual multiplication in \mathbb{Z} .

Let n=5. Draw the times table of the elements of $\mathbb{Z}_5\setminus\{\overline{0}\}$ under \otimes , i.e., calculate the products $\overline{a}\otimes\overline{b}$ for all \overline{a} and \overline{b} in $\mathbb{Z}_5\setminus\{\overline{0}\}$.

Hence, show that $\mathbb{Z}_5\setminus\{\overline{0}\}$ is closed under \otimes and possesses a neutral element for \otimes . Display the inverse of all elements in $\mathbb{Z}_5\setminus\{\overline{0}\}$ under \otimes . Conclude that $(\mathbb{Z}_5\setminus\{\overline{0}\},\otimes)$ is an Abelian group.

- c. Show that $(\mathbb{Z}_8 \setminus \{\overline{0}\}, \otimes)$ is not a group.
- d. We recall that the Bézout theorem states that two integers a and b are relatively prime (i.e., gcd(a,b)=1) if and only if there exist two integers u and v such that au+bv=1. Show that $(\mathbb{Z}_n\setminus\{\overline{0}\},\otimes)$ is a group if and only if $n\in\mathbb{N}\setminus\{0\}$ is prime.
- 2.3 Consider the set \mathcal{G} of 3×3 matrices defined as follows:

$$\mathcal{G} = \left\{ \begin{bmatrix} 1 & x & z \\ 0 & 1 & y \\ 0 & 0 & 1 \end{bmatrix} \in \mathbb{R}^{3 \times 3} \middle| x, y, z \in \mathbb{R} \right\}$$

We define \cdot as the standard matrix multiplication.

Is (\mathcal{G}, \cdot) a group? If yes, is it Abelian? Justify your answer.

2.4 Compute the following matrix products, if possible:

a.

$$\begin{bmatrix} 1 & 2 \\ 4 & 5 \\ 7 & 8 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}$$

Ъ.

$$\begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix}$$

c.

$$\begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 1 \\ 1 & 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 4 & 5 & 6 \\ 7 & 8 & 9 \end{bmatrix}$$

d.

$$\begin{bmatrix} 1 & 2 & 1 & 2 \\ 4 & 1 & -1 & -4 \end{bmatrix} \begin{bmatrix} 0 & 3 \\ 1 & -1 \\ 2 & 1 \\ 5 & 2 \end{bmatrix}$$

e.

$$\begin{bmatrix} 0 & 3 \\ 1 & -1 \\ 2 & 1 \\ 5 & 2 \end{bmatrix} \begin{bmatrix} 1 & 2 & 1 & 2 \\ 4 & 1 & -1 & -4 \end{bmatrix}$$

2.5 Find the set S of all solutions in x of the following inhomogeneous linear systems Ax = b, where A and b are defined as follows:

a.

$$\mathbf{A} = \begin{bmatrix} 1 & 1 & -1 & -1 \\ 2 & 5 & -7 & -5 \\ 2 & -1 & 1 & 3 \\ 5 & 2 & -4 & 2 \end{bmatrix}, \quad \mathbf{b} = \begin{bmatrix} 1 \\ -2 \\ 4 \\ 6 \end{bmatrix}$$

Ъ.

$$\boldsymbol{A} = \begin{bmatrix} 1 & -1 & 0 & 0 & 1 \\ 1 & 1 & 0 & -3 & 0 \\ 2 & -1 & 0 & 1 & -1 \\ -1 & 2 & 0 & -2 & -1 \end{bmatrix}, \quad \boldsymbol{b} = \begin{bmatrix} 3 \\ 6 \\ 5 \\ -1 \end{bmatrix}$$

2.6 Using Gaussian elimination, find all solutions of the inhomogeneous equation system Ax = b with

$$m{A} = egin{bmatrix} 0 & 1 & 0 & 0 & 1 & 0 \ 0 & 0 & 0 & 1 & 1 & 0 \ 0 & 1 & 0 & 0 & 0 & 1 \end{bmatrix}, \quad m{b} = egin{bmatrix} 2 \ -1 \ 1 \end{bmatrix}.$$

Find all solutions in $x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} \in \mathbb{R}^3$ of the equation system Ax = 12x,

where

$$\mathbf{A} = \begin{bmatrix} 6 & 4 & 3 \\ 6 & 0 & 9 \\ 0 & 8 & 0 \end{bmatrix}$$

and $\sum_{i=1}^{3} x_i = 1$.

Determine the inverses of the following matrices if possible: 2.8

$$\mathbf{A} = \begin{bmatrix} 2 & 3 & 4 \\ 3 & 4 & 5 \\ 4 & 5 & 6 \end{bmatrix}$$

Ъ.

$$\boldsymbol{A} = \begin{bmatrix} 1 & 0 & 1 & 0 \\ 0 & 1 & 1 & 0 \\ 1 & 1 & 0 & 1 \\ 1 & 1 & 1 & 0 \end{bmatrix}$$

Which of the following sets are subspaces of \mathbb{R}^3 ?

$$\begin{aligned} &\text{a. } A = \{(\lambda, \lambda + \mu^3, \lambda - \mu^3) \mid \lambda, \mu \in \mathbb{R}\} \\ &\text{b. } B = \{(\lambda^2, -\lambda^2, 0) \mid \lambda \in \mathbb{R}\} \end{aligned}$$

b.
$$B = \{(\lambda^2, -\lambda^2, 0) \mid \lambda \in \mathbb{R}\}\$$

c. Let γ be in \mathbb{R} .

$$C = \{ (\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3 \mid \xi_1 - 2\xi_2 + 3\xi_3 = \gamma \}$$
 d.
$$D = \{ (\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3 \mid \xi_2 \in \mathbb{Z} \}$$

d.
$$D = \{(\xi_1, \xi_2, \xi_3) \in \mathbb{R}^3 \mid \xi_2 \in \mathbb{Z}\}$$

2.10 Are the following sets of vectors linearly independent?

a.

$$m{x}_1 = egin{bmatrix} 2 \\ -1 \\ 3 \end{bmatrix}, \quad m{x}_2 = egin{bmatrix} 1 \\ 1 \\ -2 \end{bmatrix}, \quad m{x}_3 = egin{bmatrix} 3 \\ -3 \\ 8 \end{bmatrix}$$

Ъ.

$$oldsymbol{x}_1 = egin{bmatrix} 1 \ 2 \ 1 \ 0 \ 0 \end{bmatrix}, \quad oldsymbol{x}_2 = egin{bmatrix} 1 \ 1 \ 0 \ 1 \ 1 \end{bmatrix}, \quad oldsymbol{x}_3 = egin{bmatrix} 1 \ 0 \ 0 \ 1 \ 1 \end{bmatrix}$$

2.11 Write

$$\boldsymbol{y} = \begin{bmatrix} 1 \\ -2 \\ 5 \end{bmatrix}$$

as linear combination of

$$m{x}_1 = egin{bmatrix} 1 \ 1 \ 1 \end{bmatrix}, \quad m{x}_2 = egin{bmatrix} 1 \ 2 \ 3 \end{bmatrix}, \quad m{x}_3 = egin{bmatrix} 2 \ -1 \ 1 \end{bmatrix}$$

2.12 Consider two subspaces of \mathbb{R}^4 :

$$U_1 = \operatorname{span} \begin{bmatrix} 1 \\ 1 \\ -3 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ -1 \\ 0 \\ -1 \end{bmatrix}, \begin{bmatrix} -1 \\ 1 \\ -1 \\ 1 \end{bmatrix}, \quad U_2 = \operatorname{span} \begin{bmatrix} -1 \\ -2 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 2 \\ -2 \\ 0 \\ 0 \end{bmatrix}, \begin{bmatrix} -3 \\ 6 \\ -2 \\ -1 \end{bmatrix}].$$

Determine a basis of $U_1 \cap U_2$.

2.13 Consider two subspaces U_1 and U_2 , where U_1 is the solution space of the homogeneous equation system $A_1x = 0$ and U_2 is the solution space of the homogeneous equation system $A_2x = 0$ with

$$m{A}_1 = egin{bmatrix} 1 & 0 & 1 \ 1 & -2 & -1 \ 2 & 1 & 3 \ 1 & 0 & 1 \end{bmatrix}, \quad m{A}_2 = egin{bmatrix} 3 & -3 & 0 \ 1 & 2 & 3 \ 7 & -5 & 2 \ 3 & -1 & 2 \end{bmatrix}.$$

- a. Determine the dimension of U_1, U_2 .
- b. Determine bases of U_1 and U_2 .
- c. Determine a basis of $U_1 \cap U_2$.

2.14 Consider two subspaces U_1 and U_2 , where U_1 is spanned by the columns of A_1 and U_2 is spanned by the columns of A_2 with

$$\boldsymbol{A}_1 = \begin{bmatrix} 1 & 0 & 1 \\ 1 & -2 & -1 \\ 2 & 1 & 3 \\ 1 & 0 & 1 \end{bmatrix}, \quad \boldsymbol{A}_2 = \begin{bmatrix} 3 & -3 & 0 \\ 1 & 2 & 3 \\ 7 & -5 & 2 \\ 3 & -1 & 2 \end{bmatrix}.$$

- a. Determine the dimension of U_1, U_2
- b. Determine bases of U_1 and U_2
- c. Determine a basis of $U_1 \cap U_2$

2.15 Let $F = \{(x, y, z) \in \mathbb{R}^3 \mid x + y - z = 0\}$ and $G = \{(a - b, a + b, a - 3b) \mid a, b \in \mathbb{R}\}.$

- a. Show that F and G are subspaces of \mathbb{R}^3 .
- b. Calculate $F \cap G$ without resorting to any basis vector.
- c. Find one basis for F and one for G, calculate $F \cap G$ using the basis vectors previously found and check your result with the previous question.
- 2.16 Are the following mappings linear?
 - a. Let $a, b \in \mathbb{R}$.

$$\Phi:L^1([a,b])\to\mathbb{R}$$

$$f\mapsto\Phi(f)=\int_a^bf(x)dx\,,$$

where $L^1([a,b])$ denotes the set of integrable functions on [a,b].

Ъ.

$$\Phi: C^1 \to C^0$$
$$f \mapsto \Phi(f) = f',$$

where for $k \geqslant 1$, C^k denotes the set of k times continuously differentiable functions, and C^0 denotes the set of continuous functions.

c.

$$\Phi: \mathbb{R} \to \mathbb{R}$$
$$x \mapsto \Phi(x) = \cos(x)$$

d.

$$\Phi: \mathbb{R}^3 \to \mathbb{R}^2$$

$$\boldsymbol{x} \mapsto \begin{bmatrix} 1 & 2 & 3 \\ 1 & 4 & 3 \end{bmatrix} \boldsymbol{x}$$

e. Let θ be in $[0, 2\pi]$ and

$$\begin{split} \Phi: \mathbb{R}^2 &\to \mathbb{R}^2 \\ \boldsymbol{x} &\mapsto \begin{bmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{bmatrix} \boldsymbol{x} \end{split}$$

2.17 Consider the linear mapping

$$\Phi : \mathbb{R}^{3} \to \mathbb{R}^{4}$$

$$\Phi \left(\begin{bmatrix} x_{1} \\ x_{2} \\ x_{3} \end{bmatrix} \right) = \begin{bmatrix} 3x_{1} + 2x_{2} + x_{3} \\ x_{1} + x_{2} + x_{3} \\ x_{1} - 3x_{2} \\ 2x_{1} + 3x_{2} + x_{3} \end{bmatrix}$$

- Find the transformation matrix A_{Φ} .
- Determine $rk(A_{\Phi})$.
- Compute the kernel and image of Φ . What are $\dim(\ker(\Phi))$ and $\dim(\operatorname{Im}(\Phi))$?
- 2.18 Let E be a vector space. Let f and g be two automorphisms on E such that $f \circ g = \mathrm{id}_E$ (i.e., $f \circ g$ is the identity mapping id_E). Show that $\ker(f) = \ker(g \circ f)$, $\operatorname{Im}(g) = \operatorname{Im}(g \circ f)$ and that $\ker(f) \cap \operatorname{Im}(g) = \{\mathbf{0}_E\}$.
- 2.19 Consider an endomorphism $\Phi:\mathbb{R}^3\to\mathbb{R}^3$ whose transformation matrix (with respect to the standard basis in \mathbb{R}^3) is

$$m{A}_{\Phi} = egin{bmatrix} 1 & 1 & 0 \ 1 & -1 & 0 \ 1 & 1 & 1 \end{bmatrix} \,.$$

- a. Determine $\ker(\Phi)$ and $\operatorname{Im}(\Phi)$.
- b. Determine the transformation matrix $\tilde{\textbf{\textit{A}}}_{\Phi}$ with respect to the basis

$$B = (\begin{bmatrix} 1 \\ 1 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 2 \\ 1 \end{bmatrix}, \begin{bmatrix} 1 \\ 0 \\ 0 \end{bmatrix}),$$

i.e., perform a basis change toward the new basis B.

2.20 Let us consider b_1, b_2, b_1', b_2' , 4 vectors of \mathbb{R}^2 expressed in the standard basis of \mathbb{R}^2 as

$$m{b}_1 = egin{bmatrix} 2 \\ 1 \end{bmatrix}, \quad m{b}_2 = egin{bmatrix} -1 \\ -1 \end{bmatrix}, \quad m{b}_1' = egin{bmatrix} 2 \\ -2 \end{bmatrix}, \quad m{b}_2' = egin{bmatrix} 1 \\ 1 \end{bmatrix}$$

and let us define two ordered bases $B = (b_1, b_2)$ and $B' = (b'_1, b'_2)$ of \mathbb{R}^2 .

- a. Show that B and B' are two bases of \mathbb{R}^2 and draw those basis vectors.
- b. Compute the matrix P_1 that performs a basis change from B' to B.
- c. We consider c_1, c_2, c_3 , three vectors of \mathbb{R}^3 defined in the standard basis of \mathbb{R}^3 as

$$oldsymbol{c}_1 = egin{bmatrix} 1 \ 2 \ -1 \end{bmatrix}, \quad oldsymbol{c}_2 = egin{bmatrix} 0 \ -1 \ 2 \end{bmatrix}, \quad oldsymbol{c}_3 = egin{bmatrix} 1 \ 0 \ -1 \end{bmatrix}$$

and we define $C = (c_1, c_2, c_3)$.

- (i) Show that C is a basis of \mathbb{R}^3 , e.g., by using determinants (see Section 4.1).
- (ii) Let us call $C' = (c'_1, c'_2, c'_3)$ the standard basis of \mathbb{R}^3 . Determine the matrix P_2 that performs the basis change from C to C'.
- d. We consider a homomorphism $\Phi:\mathbb{R}^2\longrightarrow\mathbb{R}^3$, such that

$$\Phi(\mathbf{b}_1 + \mathbf{b}_2) = \mathbf{c}_2 + \mathbf{c}_3
\Phi(\mathbf{b}_1 - \mathbf{b}_2) = 2\mathbf{c}_1 - \mathbf{c}_2 + 3\mathbf{c}_3$$

where $B = (\boldsymbol{b}_1, \boldsymbol{b}_2)$ and $C = (\boldsymbol{c}_1, \boldsymbol{c}_2, \boldsymbol{c}_3)$ are ordered bases of \mathbb{R}^2 and \mathbb{R}^3 , respectively.

Determine the transformation matrix ${\bf A}_\Phi$ of Φ with respect to the ordered bases ${\cal B}$ and ${\cal C}.$

- e. Determine A', the transformation matrix of Φ with respect to the bases B' and C'.
- f. Let us consider the vector $\mathbf{x} \in \mathbb{R}^2$ whose coordinates in B' are $[2,3]^{\top}$. In other words, $\mathbf{x} = 2b_1' + 3b_2'$.
 - (i) Calculate the coordinates of x in B.
 - (ii) Based on that, compute the coordinates of $\Phi(x)$ expressed in C.
 - (iii) Then, write $\Phi(x)$ in terms of c'_1, c'_2, c'_3 .
 - (iv) Use the representation of x in B' and the matrix A' to find this result directly.