Linear Algebra

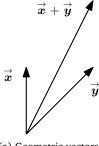


When formalizing intuitive concepts, a common approach is to construct a set of objects (symbols) and a set of rules to manipulate these objects. This is known as an algebra. Linear algebra is the study of vectors and certain rules to manipulate vectors. The vectors many of us know from school are called "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 \vec{x} , \vec{y} can be added, such that $\vec{x} + \vec{y} = \vec{z}$ is another geometric vector. Furthermore, multiplication by a scalar $\lambda \vec{x}, \lambda \in \mathbb{R}$, 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





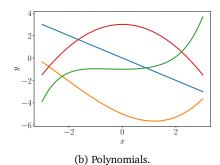


Figure 2.1 Different types of vectors. Vectors can be surprising objects, including (a) geometric vectors and (b) polynomials.

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

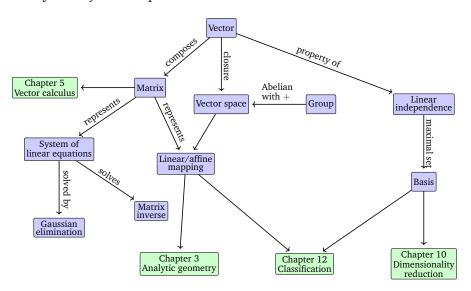


Figure 2.2 A mind map of the concepts introduced in this chapter, along with where they are used in other parts of the book.

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)



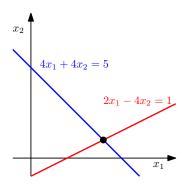


Figure 2.3 The solution space of a system of two linear equations with two variables can be geometrically interpreted as the intersection of two lines. Every linear equation represents a line.

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. $A \in \mathbb{R}^{m \times n}$ can be equivalently represented as $a \in \mathbb{R}^{mn}$ 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.,

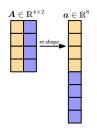
$$\mathbf{A} + \mathbf{B} := \begin{bmatrix} a_{11} + b_{11} & \cdots & a_{1n} + b_{1n} \\ \vdots & & \vdots \\ a_{m1} + b_{m1} & \cdots & a_{mn} + b_{mn} \end{bmatrix} \in \mathbb{R}^{m \times n}.$$
 (2.12)

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

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

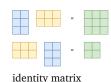
$$\boldsymbol{B}\boldsymbol{A} = \begin{bmatrix} 0 & 2 \\ 1 & -1 \\ 0 & 1 \end{bmatrix} \begin{bmatrix} 1 & 2 & 3 \\ 3 & 2 & 1 \end{bmatrix} = \begin{bmatrix} 6 & 4 & 2 \\ -2 & 0 & 2 \\ 3 & 2 & 1 \end{bmatrix} \in \mathbb{R}^{3 \times 3}.$$
 (2.16)

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.

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

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

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)