

Figure 3.3 For different norms, the red lines indicate the set of vectors with norm 1. Left: Manhattan norm; Right: Euclidean distance.

3.1 Norms

When we think of geometric vectors, i.e., directed line segments that start at the origin, then intuitively the length of a vector is the distance of the "end" of this directed line segment from the origin. In the following, we will discuss the notion of the length of vectors using the concept of a norm.

Definition 3.1 (Norm). A *norm* on a vector space V is a function

norm

$$\|\cdot\|:V\to\mathbb{R}\,,\tag{3.1}$$

$$x \mapsto \|x\|$$
, (3.2)

which assigns each vector x its *length* $||x|| \in \mathbb{R}$, such that for all $\lambda \in \mathbb{R}$ and $x, y \in V$ the following hold:

length

• Absolutely homogeneous: $\|\lambda x\| = |\lambda| \|x\|$

lacksquare Triangle inequality: $\|x+y\| \leqslant \|x\| + \|y\|$

• Positive definite: $||x|| \geqslant 0$ and $||x|| = 0 \iff x = 0$

absolutely homogeneous triangle inequality positive definite

In geometric terms, the triangle inequality states that for any triangle, the sum of the lengths of any two sides must be greater than or equal to the length of the remaining side; see Figure 3.2 for an illustration. Definition 3.1 is in terms of a general vector space V (Section 2.4), but in this book we will only consider a finite-dimensional vector space \mathbb{R}^n . Recall that for a vector $\boldsymbol{x} \in \mathbb{R}^n$ we denote the elements of the vector using a subscript, that is, x_i is the i^{th} element of the vector \boldsymbol{x} .

Figure 3.2 Triangle inequality.



Example 3.1 (Manhattan Norm)

The *Manhattan norm* on \mathbb{R}^n is defined for $\boldsymbol{x} \in \mathbb{R}^n$ as

Manhattan norm

$$\|\boldsymbol{x}\|_1 := \sum_{i=1}^n |x_i|,$$
 (3.3)

where $|\cdot|$ is the absolute value. The left panel of Figure 3.3 shows all vectors $x \in \mathbb{R}^2$ with $||x||_1 = 1$. The Manhattan norm is also called ℓ_1 norm.

 ℓ_1 norm

Euclidean norm

Example 3.2 (Euclidean Norm)

The Euclidean norm of $\boldsymbol{x} \in \mathbb{R}^n$ is defined as

$$\|x\|_2 := \sqrt{\sum_{i=1}^n x_i^2} = \sqrt{x^\top x}$$
 (3.4)

Euclidean distance

 ℓ_2 norm

and computes the *Euclidean distance* of x from the origin. The right panel of Figure 3.3 shows all vectors $x \in \mathbb{R}^2$ with $||x||_2 = 1$. The Euclidean norm is also called ℓ_2 norm.

Remark. Throughout this book, we will use the Euclidean norm (3.4) by default if not stated otherwise.

3.2 Inner Products

Inner products allow for the introduction of intuitive geometrical concepts, such as the length of a vector and the angle or distance between two vectors. A major purpose of inner products is to determine whether vectors are orthogonal to each other.

3.2.1 Dot Product

scalar product dot product We may already be familiar with a particular type of inner product, the *scalar product/dot product* in \mathbb{R}^n , which is given by

$$\boldsymbol{x}^{\top}\boldsymbol{y} = \sum_{i=1}^{n} x_{i} y_{i} . \tag{3.5}$$

We will refer to this particular inner product as the dot product in this book. However, inner products are more general concepts with specific properties, which we will now introduce.

3.2.2 General Inner Products

bilinear mapping

Recall the linear mapping from Section 2.7, where we can rearrange the mapping with respect to addition and multiplication with a scalar. A bilinear mapping Ω is a mapping with two arguments, and it is linear in each argument, i.e., when we look at a vector space V then it holds that for all $x, y, z \in V$, $\lambda, \psi \in \mathbb{R}$ that

$$\Omega(\lambda x + \psi y, z) = \lambda \Omega(x, z) + \psi \Omega(y, z)$$
(3.6)

$$\Omega(\mathbf{x}, \lambda \mathbf{y} + \psi \mathbf{z}) = \lambda \Omega(\mathbf{x}, \mathbf{y}) + \psi \Omega(\mathbf{x}, \mathbf{z}). \tag{3.7}$$

Here, (3.6) asserts that Ω is linear in the first argument, and (3.7) asserts that Ω is linear in the second argument (see also (2.87)).

Definition 3.2. Let V be a vector space and $\Omega: V \times V \to \mathbb{R}$ be a bilinear mapping that takes two vectors and maps them onto a real number. Then

• Ω is called *symmetric* if $\Omega(x, y) = \Omega(y, x)$ for all $x, y \in V$, i.e., the order of the arguments does not matter.

symmetric

• Ω is called *positive definite* if

positive definite

$$\forall \boldsymbol{x} \in V \setminus \{\boldsymbol{0}\} : \Omega(\boldsymbol{x}, \boldsymbol{x}) > 0, \quad \Omega(\boldsymbol{0}, \boldsymbol{0}) = 0.$$
 (3.8)

Definition 3.3. Let V be a vector space and $\Omega: V \times V \to \mathbb{R}$ be a bilinear mapping that takes two vectors and maps them onto a real number. Then

- A positive definite, symmetric bilinear mapping $\Omega: V \times V \to \mathbb{R}$ is called an *inner product* on V. We typically write $\langle x, y \rangle$ instead of $\Omega(x, y)$.
- The pair $(V, \langle \cdot, \cdot \rangle)$ is called an *inner product space* or (real) *vector space* with inner product. If we use the dot product defined in (3.5), we call $(V, \langle \cdot, \cdot \rangle)$ a *Euclidean vector space*.

inner product inner product space vector space with inner product Euclidean vector space

We will refer to these spaces as inner product spaces in this book.

Example 3.3 (Inner Product That Is Not the Dot Product)

Consider $V = \mathbb{R}^2$. If we define

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle := x_1 y_1 - (x_1 y_2 + x_2 y_1) + 2x_2 y_2$$
 (3.9)

then $\langle \cdot, \cdot \rangle$ is an inner product but different from the dot product. The proof will be an exercise.

3.2.3 Symmetric, Positive Definite Matrices

Symmetric, positive definite matrices play an important role in machine learning, and they are defined via the inner product. In Section 4.3, we will return to symmetric, positive definite matrices in the context of matrix decompositions. The idea of symmetric positive semidefinite matrices is key in the definition of kernels (Section 12.4).

Consider an n-dimensional vector space V with an inner product $\langle \cdot, \cdot \rangle$: $V \times V \to \mathbb{R}$ (see Definition 3.3) and an ordered basis $B = (\boldsymbol{b}_1, \dots, \boldsymbol{b}_n)$ of V. Recall from Section 2.6.1 that any vectors $\boldsymbol{x}, \boldsymbol{y} \in V$ can be written as linear combinations of the basis vectors so that $\boldsymbol{x} = \sum_{i=1}^n \psi_i \boldsymbol{b}_i \in V$ and $\boldsymbol{y} = \sum_{j=1}^n \lambda_j \boldsymbol{b}_j \in V$ for suitable $\psi_i, \lambda_j \in \mathbb{R}$. Due to the bilinearity of the inner product, it holds for all $\boldsymbol{x}, \boldsymbol{y} \in V$ that

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \left\langle \sum_{i=1}^{n} \psi_{i} \boldsymbol{b}_{i}, \sum_{j=1}^{n} \lambda_{j} \boldsymbol{b}_{j} \right\rangle = \sum_{i=1}^{n} \sum_{j=1}^{n} \psi_{i} \left\langle \boldsymbol{b}_{i}, \boldsymbol{b}_{j} \right\rangle \lambda_{j} = \hat{\boldsymbol{x}}^{\top} \boldsymbol{A} \hat{\boldsymbol{y}}, \quad (3.10)$$

where $A_{ij} := \langle \boldsymbol{b}_i, \boldsymbol{b}_j \rangle$ and $\hat{\boldsymbol{x}}, \hat{\boldsymbol{y}}$ are the coordinates of \boldsymbol{x} and \boldsymbol{y} with respect to the basis B. This implies that the inner product $\langle \cdot, \cdot \rangle$ is uniquely determined through \boldsymbol{A} . The symmetry of the inner product also means that \boldsymbol{A}

is symmetric. Furthermore, the positive definiteness of the inner product implies that

$$\forall \boldsymbol{x} \in V \setminus \{\boldsymbol{0}\} : \boldsymbol{x}^{\top} \boldsymbol{A} \boldsymbol{x} > 0. \tag{3.11}$$

Definition 3.4 (Symmetric, Positive Definite Matrix). A symmetric matrix $A \in \mathbb{R}^{n \times n}$ that satisfies (3.11) is called symmetric, positive definite, or just positive definite. If only \geqslant holds in (3.11), then A is called symmetric, positive semidefinite.

symmetric, positive definite positive definite symmetric, positive semidefinite

Example 3.4 (Symmetric, Positive Definite Matrices)

Consider the matrices

$$\mathbf{A}_1 = \begin{bmatrix} 9 & 6 \\ 6 & 5 \end{bmatrix}, \quad \mathbf{A}_2 = \begin{bmatrix} 9 & 6 \\ 6 & 3 \end{bmatrix}. \tag{3.12}$$

 A_1 is positive definite because it is symmetric and

$$\boldsymbol{x}^{\top} \boldsymbol{A}_{1} \boldsymbol{x} = \begin{bmatrix} x_{1} & x_{2} \end{bmatrix} \begin{bmatrix} 9 & 6 \\ 6 & 5 \end{bmatrix} \begin{bmatrix} x_{1} \\ x_{2} \end{bmatrix}$$
(3.13a)

$$=9x_1^2 + 12x_1x_2 + 5x_2^2 = (3x_1 + 2x_2)^2 + x_2^2 > 0$$
 (3.13b)

for all ${m x} \in V \backslash \{{m 0}\}.$ In contrast, ${m A}_2$ is symmetric but not positive definite because $\mathbf{x}^{\top} \mathbf{A}_2 \mathbf{x} = 9x_1^2 + 12x_1x_2 + 3x_2^2 = (3x_1 + 2x_2)^2 - x_2^2$ can be less than 0, e.g., for $x = [2, -3]^{\top}$.

If $A \in \mathbb{R}^{n \times n}$ is symmetric, positive definite, then

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \hat{\boldsymbol{x}}^{\top} A \hat{\boldsymbol{y}} \tag{3.14}$$

defines an inner product with respect to an ordered basis B, where \hat{x} and \hat{y} are the coordinate representations of $x, y \in V$ with respect to B.

Theorem 3.5. For a real-valued, finite-dimensional vector space V and an ordered basis B of V, it holds that $\langle \cdot, \cdot \rangle : V \times V \to \mathbb{R}$ is an inner product if and only if there exists a symmetric, positive definite matrix $A \in \mathbb{R}^{n \times n}$ with

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \hat{\boldsymbol{x}}^{\top} A \hat{\boldsymbol{y}}. \tag{3.15}$$

The following properties hold if $A \in \mathbb{R}^{n \times n}$ is symmetric and positive definite:

- lacksquare The null space (kernel) of $m{A}$ consists only of $m{0}$ because $m{x}^{ op} m{A} m{x} > 0$ for all $x \neq 0$. This implies that $Ax \neq 0$ if $x \neq 0$.
- The diagonal elements a_{ii} of A are positive because $a_{ii} = e_i^{\top} A e_i > 0$, where e_i is the *i*th vector of the standard basis in \mathbb{R}^n .

3.3 Lengths and Distances

In Section 3.1, we already discussed norms that we can use to compute the length of a vector. Inner products and norms are closely related in the sense that any inner product induces a norm

Inner products induce norms.

$$\|\boldsymbol{x}\| := \sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle} \tag{3.16}$$

in a natural way, such that we can compute lengths of vectors using the inner product. However, not every norm is induced by an inner product. The Manhattan norm (3.3) is an example of a norm without a corresponding inner product. In the following, we will focus on norms that are induced by inner products and introduce geometric concepts, such as lengths, distances, and angles.

Remark (Cauchy-Schwarz Inequality). For an inner product vector space $(V, \langle \cdot, \cdot \rangle)$ the induced norm $\| \cdot \|$ satisfies the *Cauchy-Schwarz inequality*

Cauchy-Schwarz inequality

$$|\langle x, y \rangle| \leqslant ||x|| ||y||. \tag{3.17}$$



Example 3.5 (Lengths of Vectors Using Inner Products)

In geometry, we are often interested in lengths of vectors. We can now use an inner product to compute them using (3.16). Let us take $x = [1, 1]^T \in \mathbb{R}^2$. If we use the dot product as the inner product, with (3.16) we obtain

$$\|\mathbf{x}\| = \sqrt{\mathbf{x}^{\top}\mathbf{x}} = \sqrt{1^2 + 1^2} = \sqrt{2}$$
 (3.18)

as the length of x. Let us now choose a different inner product:

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle := \boldsymbol{x}^{\top} \begin{bmatrix} 1 & -\frac{1}{2} \\ -\frac{1}{2} & 1 \end{bmatrix} \boldsymbol{y} = x_1 y_1 - \frac{1}{2} (x_1 y_2 + x_2 y_1) + x_2 y_2.$$
 (3.19)

If we compute the norm of a vector, then this inner product returns smaller values than the dot product if x_1 and x_2 have the same sign (and $x_1x_2 > 0$); otherwise, it returns greater values than the dot product. With this inner product, we obtain

$$\langle \boldsymbol{x}, \boldsymbol{x} \rangle = x_1^2 - x_1 x_2 + x_2^2 = 1 - 1 + 1 = 1 \implies \|\boldsymbol{x}\| = \sqrt{1} = 1, \quad (3.20)$$

such that *x* is "shorter" with this inner product than with the dot product.

Definition 3.6 (Distance and Metric). Consider an inner product space $(V,\langle\cdot,\cdot\rangle)$. Then

$$d(\boldsymbol{x}, \boldsymbol{y}) := \|\boldsymbol{x} - \boldsymbol{y}\| = \sqrt{\langle \boldsymbol{x} - \boldsymbol{y}, \boldsymbol{x} - \boldsymbol{y} \rangle}$$
(3.21)

is called the *distance* between x and y for $x, y \in V$. If we use the dot product as the inner product, then the distance is called *Euclidean distance*.

distance Euclidean distance

The mapping

$$d: V \times V \to \mathbb{R} \tag{3.22}$$

$$(\boldsymbol{x}, \boldsymbol{y}) \mapsto d(\boldsymbol{x}, \boldsymbol{y})$$
 (3.23)

metric

is called a metric.

Remark. Similar to the length of a vector, the distance between vectors does not require an inner product: a norm is sufficient. If we have a norm induced by an inner product, the distance may vary depending on the choice of the inner product.

A metric *d* satisfies the following:

positive definite

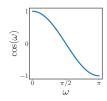
1. d is positive definite, i.e., $d(x,y) \geqslant 0$ for all $x,y \in V$ and $d(x,y) = 0 \iff x = y$.

symmetric triangle inequality

- 2. d is symmetric, i.e., d(x, y) = d(y, x) for all $x, y \in V$.
- 3. Triangle inequality: $d(x, z) \le d(x, y) + d(y, z)$ for all $x, y, z \in V$.

Remark. At first glance, the lists of properties of inner products and metrics look very similar. However, by comparing Definition 3.3 with Definition 3.6 we observe that $\langle x, y \rangle$ and d(x, y) behave in opposite directions. Very similar x and y will result in a large value for the inner product and a small value for the metric.

Figure 3.4 When restricted to $[0,\pi]$ then $f(\omega)=\cos(\omega)$ returns a unique number in the interval [-1,1].



3.4 Angles and Orthogonality

In addition to enabling the definition of lengths of vectors, as well as the distance between two vectors, inner products also capture the geometry of a vector space by defining the angle ω between two vectors. We use the Cauchy-Schwarz inequality (3.17) to define angles ω in inner product spaces between two vectors x, y, and this notion coincides with our intuition in \mathbb{R}^2 and \mathbb{R}^3 . Assume that $x \neq 0, y \neq 0$. Then

$$-1 \leqslant \frac{\langle \boldsymbol{x}, \boldsymbol{y} \rangle}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|} \leqslant 1. \tag{3.24}$$

Therefore, there exists a unique $\omega \in [0, \pi]$, illustrated in Figure 3.4, with

$$\cos \omega = \frac{\langle \boldsymbol{x}, \boldsymbol{y} \rangle}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|}.$$
 (3.25)

angle

The number ω is the *angle* between the vectors \boldsymbol{x} and \boldsymbol{y} . Intuitively, the angle between two vectors tells us how similar their orientations are. For example, using the dot product, the angle between \boldsymbol{x} and $\boldsymbol{y}=4\boldsymbol{x}$, i.e., \boldsymbol{y} is a scaled version of \boldsymbol{x} , is 0: Their orientation is the same.

Example 3.6 (Angle between Vectors)

Let us compute the angle between $\boldsymbol{x} = [1,1]^{\top} \in \mathbb{R}^2$ and $\boldsymbol{y} = [1,2]^{\top} \in \mathbb{R}^2$; see Figure 3.5, where we use the dot product as the inner product. Then we get

$$\cos \omega = \frac{\langle \boldsymbol{x}, \boldsymbol{y} \rangle}{\sqrt{\langle \boldsymbol{x}, \boldsymbol{x} \rangle \langle \boldsymbol{y}, \boldsymbol{y} \rangle}} = \frac{\boldsymbol{x}^{\top} \boldsymbol{y}}{\sqrt{\boldsymbol{x}^{\top} \boldsymbol{x} \boldsymbol{y}^{\top} \boldsymbol{y}}} = \frac{3}{\sqrt{10}}, \quad (3.26)$$

and the angle between the two vectors is $\arccos(\frac{3}{\sqrt{10}})\approx 0.32\,\mathrm{rad}$, which corresponds to about 18° .

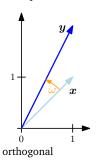
A key feature of the inner product is that it also allows us to characterize vectors that are orthogonal.

Definition 3.7 (Orthogonality). Two vectors x and y are *orthogonal* if and only if $\langle x, y \rangle = 0$, and we write $x \perp y$. If additionally ||x|| = 1 = ||y||, i.e., the vectors are unit vectors, then x and y are *orthonormal*.

An implication of this definition is that the **0**-vector is orthogonal to every vector in the vector space.

Remark. Orthogonality is the generalization of the concept of perpendicularity to bilinear forms that do not have to be the dot product. In our context, geometrically, we can think of orthogonal vectors as having a right angle with respect to a specific inner product.

Figure 3.5 The angle ω between two vectors $\boldsymbol{x}, \boldsymbol{y}$ is computed using the inner product.



orthonormal

Example 3.7 (Orthogonal Vectors)

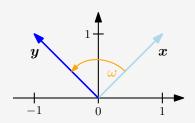


Figure 3.6 The angle ω between two vectors $\boldsymbol{x}, \boldsymbol{y}$ can change depending on the inner product.

Consider two vectors $\boldsymbol{x} = [1,1]^{\top}, \boldsymbol{y} = [-1,1]^{\top} \in \mathbb{R}^2$; see Figure 3.6. We are interested in determining the angle ω between them using two different inner products. Using the dot product as the inner product yields an angle ω between \boldsymbol{x} and \boldsymbol{y} of 90° , such that $\boldsymbol{x} \perp \boldsymbol{y}$. However, if we choose the inner product

$$\langle \boldsymbol{x}, \boldsymbol{y} \rangle = \boldsymbol{x}^{\top} \begin{bmatrix} 2 & 0 \\ 0 & 1 \end{bmatrix} \boldsymbol{y},$$
 (3.27)

we get that the angle ω between x and y is given by

$$\cos \omega = \frac{\langle \boldsymbol{x}, \boldsymbol{y} \rangle}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|} = -\frac{1}{3} \implies \omega \approx 1.91 \,\mathrm{rad} \approx 109.5^{\circ},$$
 (3.28)

and x and y are not orthogonal. Therefore, vectors that are orthogonal with respect to one inner product do not have to be orthogonal with respect to a different inner product.

orthogonal matrix

Definition 3.8 (Orthogonal Matrix). A square matrix $A \in \mathbb{R}^{n \times n}$ is an *orthogonal matrix* if and only if its columns are orthonormal so that

$$AA^{\top} = I = A^{\top}A, \qquad (3.29)$$

which implies that

$$\boldsymbol{A}^{-1} = \boldsymbol{A}^{\top} \,. \tag{3.30}$$

i.e., the inverse is obtained by simply transposing the matrix.

Transformations by orthogonal matrices are special because the length of a vector x is not changed when transforming it using an orthogonal matrix A. For the dot product, we obtain

$$\|Ax\|^2 = (Ax)^{\top}(Ax) = x^{\top}A^{\top}Ax = x^{\top}Ix = x^{\top}x = \|x\|^2$$
. (3.31)

Moreover, the angle between any two vectors x, y, as measured by their inner product, is also unchanged when transforming both of them using an orthogonal matrix A. Assuming the dot product as the inner product, the angle of the images Ax and Ay is given as

$$\cos \omega = \frac{(A\boldsymbol{x})^{\top}(A\boldsymbol{y})}{\|A\boldsymbol{x}\| \|A\boldsymbol{y}\|} = \frac{\boldsymbol{x}^{\top} \boldsymbol{A}^{\top} A \boldsymbol{y}}{\sqrt{\boldsymbol{x}^{\top} \boldsymbol{A}^{\top} A \boldsymbol{x} \boldsymbol{y}^{\top} \boldsymbol{A}^{\top} A \boldsymbol{y}}} = \frac{\boldsymbol{x}^{\top} \boldsymbol{y}}{\|\boldsymbol{x}\| \|\boldsymbol{y}\|}, \quad (3.32)$$

which gives exactly the angle between x and y. This means that orthogonal matrices A with $A^{\top} = A^{-1}$ preserve both angles and distances. It turns out that orthogonal matrices define transformations that are rotations (with the possibility of flips). In Section 3.9, we will discuss more details about rotations.

3.5 Orthonormal Basis

In Section 2.6.1, we characterized properties of basis vectors and found that in an n-dimensional vector space, we need n basis vectors, i.e., n vectors that are linearly independent. In Sections 3.3 and 3.4, we used inner products to compute the length of vectors and the angle between vectors. In the following, we will discuss the special case where the basis vectors are orthogonal to each other and where the length of each basis vector is 1. We will call this basis then an orthonormal basis.

It is convention to call these matrices "orthogonal" but a more precise description would be "orthonormal". Transformations with orthogonal matrices preserve distances and angles.