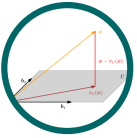
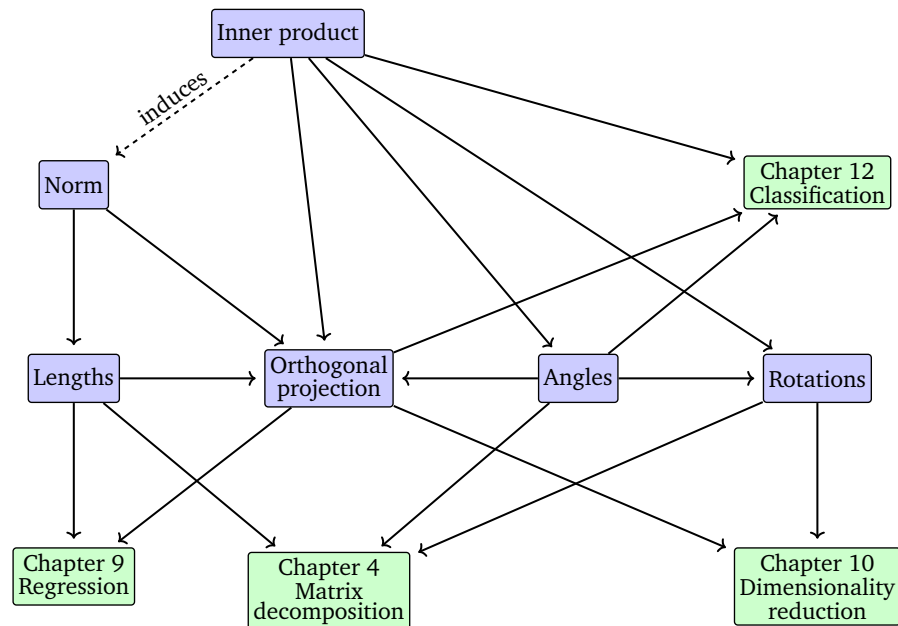


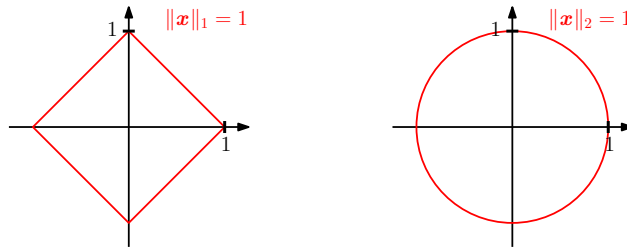
## Analytic Geometry



In Chapter 2, we studied vectors, vector spaces, and linear mappings at a general but abstract level. In this chapter, we will add some geometric interpretation and intuition to all of these concepts. In particular, we will look at geometric vectors and compute their lengths and distances or angles between two vectors. To be able to do this, we equip the vector space with an inner product that induces the geometry of the vector space. Inner products and their corresponding norms and metrics capture the intuitive notions of similarity and distances, which we use to develop the support vector machine in Chapter 12. We will then use the concepts of lengths and angles between vectors to discuss orthogonal projections, which will play a central role when we discuss principal component analysis in Chapter 10 and regression via maximum likelihood estimation in Chapter 9. Figure 3.1 gives an overview of how concepts in this chapter are related and how they are connected to other chapters of the book.

**Figure 3.1** A mind map of the concepts introduced in this chapter, along with when they are used in other parts of the book.





**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

$$\|\cdot\| : V \rightarrow \mathbb{R}, \quad (3.1)$$

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

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:*  $\|\lambda x\| = |\lambda| \|x\|$
- *Triangle inequality:*  $\|x + y\| \leq \|x\| + \|y\|$
- *Positive definite:*  $\|x\| \geq 0$  and  $\|x\| = 0 \iff x = 0$

absolutely

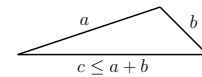
homogeneous

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  $x \in \mathbb{R}^n$  we denote the elements of the vector using a subscript, that is,  $x_i$  is the  $i^{\text{th}}$  element of the vector  $x$ .

**Figure 3.2** Triangle inequality.



#### Example 3.1 (Manhattan Norm)

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

Manhattan norm

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

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  $\ell_1$  norm.

$\ell_1$  norm

**Example 3.2 (Euclidean Norm)**

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

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

and computes the *Euclidean distance* of  $\mathbf{x}$  from the origin. The right panel of Figure 3.3 shows all vectors  $\mathbf{x} \in \mathbb{R}^2$  with  $\|\mathbf{x}\|_2 = 1$ . The Euclidean norm is also called  $\ell_2$  norm.

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

**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**

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

$$\mathbf{x}^\top \mathbf{y} = \sum_{i=1}^n x_i y_i. \quad (3.5)$$

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**

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*  $\Omega$  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  $\mathbf{x}, \mathbf{y}, \mathbf{z} \in V$ ,  $\lambda, \psi \in \mathbb{R}$  that

$$\Omega(\lambda \mathbf{x} + \psi \mathbf{y}, \mathbf{z}) = \lambda \Omega(\mathbf{x}, \mathbf{z}) + \psi \Omega(\mathbf{y}, \mathbf{z}) \quad (3.6)$$

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

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

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

- $\Omega$  is called *symmetric* if  $\Omega(\mathbf{x}, \mathbf{y}) = \Omega(\mathbf{y}, \mathbf{x})$  for all  $\mathbf{x}, \mathbf{y} \in V$ , i.e., the order of the arguments does not matter. symmetric
- $\Omega$  is called *positive definite* if positive definite

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

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

- A positive definite, symmetric bilinear mapping  $\Omega : V \times V \rightarrow \mathbb{R}$  is called an *inner product* on  $V$ . We typically write  $\langle \mathbf{x}, \mathbf{y} \rangle$  instead of  $\Omega(\mathbf{x}, \mathbf{y})$ . inner product
- 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 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

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

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

$$\langle \mathbf{x}, \mathbf{y} \rangle = \left\langle \sum_{i=1}^n \psi_i \mathbf{b}_i, \sum_{j=1}^n \lambda_j \mathbf{b}_j \right\rangle = \sum_{i=1}^n \sum_{j=1}^n \psi_i \langle \mathbf{b}_i, \mathbf{b}_j \rangle \lambda_j = \hat{\mathbf{x}}^\top \mathbf{A} \hat{\mathbf{y}}, \quad (3.10)$$

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

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

$$\forall \mathbf{x} \in V \setminus \{\mathbf{0}\} : \mathbf{x}^\top \mathbf{A} \mathbf{x} > 0. \quad (3.11)$$

symmetric, positive  
definite  
positive definite  
symmetric, positive  
semidefinite

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

**Example 3.4 (Symmetric, Positive Definite Matrices)**

Consider the matrices

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

$\mathbf{A}_1$  is positive definite because it is symmetric and

$$\mathbf{x}^\top \mathbf{A}_1 \mathbf{x} = \begin{bmatrix} x_1 & x_2 \end{bmatrix} \begin{bmatrix} 9 & 6 \\ 6 & 5 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \end{bmatrix} \quad (3.13a)$$

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

for all  $\mathbf{x} \in V \setminus \{\mathbf{0}\}$ . In contrast,  $\mathbf{A}_2$  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  $\mathbf{x} = [2, -3]^\top$ .

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

$$\langle \mathbf{x}, \mathbf{y} \rangle = \hat{\mathbf{x}}^\top \mathbf{A} \hat{\mathbf{y}} \quad (3.14)$$

defines an inner product with respect to an ordered basis  $B$ , where  $\hat{\mathbf{x}}$  and  $\hat{\mathbf{y}}$  are the coordinate representations of  $\mathbf{x}, \mathbf{y} \in V$  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  $\langle \cdot, \cdot \rangle : V \times V \rightarrow \mathbb{R}$  is an inner product if and only if there exists a symmetric, positive definite matrix  $\mathbf{A} \in \mathbb{R}^{n \times n}$  with

$$\langle \mathbf{x}, \mathbf{y} \rangle = \hat{\mathbf{x}}^\top \mathbf{A} \hat{\mathbf{y}}. \quad (3.15)$$

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

- The null space (kernel) of  $\mathbf{A}$  consists only of  $\mathbf{0}$  because  $\mathbf{x}^\top \mathbf{A} \mathbf{x} > 0$  for all  $\mathbf{x} \neq \mathbf{0}$ . This implies that  $\mathbf{A} \mathbf{x} \neq \mathbf{0}$  if  $\mathbf{x} \neq \mathbf{0}$ .
- The diagonal elements  $a_{ii}$  of  $\mathbf{A}$  are positive because  $a_{ii} = \mathbf{e}_i^\top \mathbf{A} \mathbf{e}_i > 0$ , where  $\mathbf{e}_i$  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.

$$\|x\| := \sqrt{\langle x, x \rangle} \quad (3.16)$$

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

$$|\langle x, y \rangle| \leq \|x\| \|y\|. \quad (3.17)$$

◇

#### 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  $x = [1, 1]^\top \in \mathbb{R}^2$ . If we use the dot product as the inner product, with (3.16) we obtain

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

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

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

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  $x_1 x_2 > 0$ ); otherwise, it returns greater values than the dot product. With this inner product, we obtain

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

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

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

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

$$d : V \times V \rightarrow \mathbb{R} \quad (3.22)$$

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

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.  $\diamond$

A metric  $d$  satisfies the following:

positive definite

1.  $d$  is *positive definite*, i.e.,  $d(\mathbf{x}, \mathbf{y}) \geq 0$  for all  $\mathbf{x}, \mathbf{y} \in V$  and  $d(\mathbf{x}, \mathbf{y}) = 0 \iff \mathbf{x} = \mathbf{y}$ .

symmetric

2.  $d$  is *symmetric*, i.e.,  $d(\mathbf{x}, \mathbf{y}) = d(\mathbf{y}, \mathbf{x})$  for all  $\mathbf{x}, \mathbf{y} \in V$ .

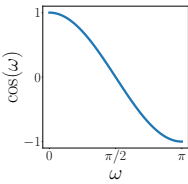
triangle inequality

3. *Triangle inequality*:  $d(\mathbf{x}, \mathbf{z}) \leq d(\mathbf{x}, \mathbf{y}) + d(\mathbf{y}, \mathbf{z})$  for all  $\mathbf{x}, \mathbf{y}, \mathbf{z} \in V$ .

*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  $\langle \mathbf{x}, \mathbf{y} \rangle$  and  $d(\mathbf{x}, \mathbf{y})$  behave in opposite directions. Very similar  $\mathbf{x}$  and  $\mathbf{y}$  will result in a large value for the inner product and a small value for the metric.  $\diamond$

### 3.4 Angles and Orthogonality

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



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  $\omega$  between two vectors. We use the Cauchy-Schwarz inequality (3.17) to define angles  $\omega$  in inner product spaces between two vectors  $\mathbf{x}, \mathbf{y}$ , and this notion coincides with our intuition in  $\mathbb{R}^2$  and  $\mathbb{R}^3$ . Assume that  $\mathbf{x} \neq \mathbf{0}, \mathbf{y} \neq \mathbf{0}$ . Then

$$-1 \leq \frac{\langle \mathbf{x}, \mathbf{y} \rangle}{\|\mathbf{x}\| \|\mathbf{y}\|} \leq 1. \quad (3.24)$$

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

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

angle

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

**Example 3.6 (Angle between Vectors)**

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

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

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

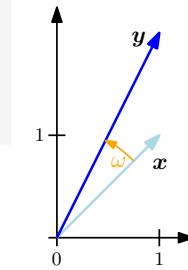
A key feature of the inner product is that it also allows us to characterize vectors that are orthogonal.

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

An implication of this definition is that the  $\mathbf{0}$ -vector is orthogonal to every vector in the vector space.

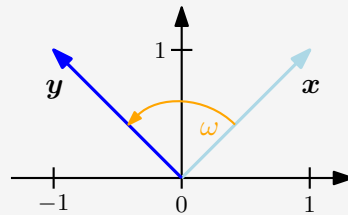
*Remark.* Orthogonality is the generalization of the concept of perpendicularity to bilinear forms that do not have to be the dot product. In our context, geometrically, we can think of orthogonal vectors as having a right angle with respect to a specific inner product.  $\diamond$

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



orthogonal

orthonormal

**Example 3.7 (Orthogonal Vectors)**

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

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

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



we get that the angle  $\omega$  between  $\mathbf{x}$  and  $\mathbf{y}$  is given by

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

and  $\mathbf{x}$  and  $\mathbf{y}$  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  $\mathbf{A} \in \mathbb{R}^{n \times n}$  is an *orthogonal matrix* if and only if its columns are orthonormal so that

$$\mathbf{A}\mathbf{A}^\top = \mathbf{I} = \mathbf{A}^\top \mathbf{A}, \quad (3.29)$$

which implies that

$$\mathbf{A}^{-1} = \mathbf{A}^\top, \quad (3.30)$$

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

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

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

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

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

which gives exactly the angle between  $\mathbf{x}$  and  $\mathbf{y}$ . This means that orthogonal matrices  $\mathbf{A}$  with  $\mathbf{A}^\top = \mathbf{A}^{-1}$  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.

Let us introduce this more formally.

**Definition 3.9** (Orthonormal Basis). Consider an  $n$ -dimensional vector space  $V$  and a basis  $\{\mathbf{b}_1, \dots, \mathbf{b}_n\}$  of  $V$ . If

$$\langle \mathbf{b}_i, \mathbf{b}_j \rangle = 0 \quad \text{for } i \neq j \quad (3.33)$$

$$\langle \mathbf{b}_i, \mathbf{b}_i \rangle = 1 \quad (3.34)$$

for all  $i, j = 1, \dots, n$  then the basis is called an *orthonormal basis* (ONB). If only (3.33) is satisfied, then the basis is called an *orthogonal basis*. Note that (3.34) implies that every basis vector has length/norm 1.

orthonormal basis  
ONB  
orthogonal basis

Recall from Section 2.6.1 that we can use Gaussian elimination to find a basis for a vector space spanned by a set of vectors. Assume we are given a set  $\{\tilde{\mathbf{b}}_1, \dots, \tilde{\mathbf{b}}_n\}$  of non-orthogonal and unnormalized basis vectors. We concatenate them into a matrix  $\tilde{\mathbf{B}} = [\tilde{\mathbf{b}}_1, \dots, \tilde{\mathbf{b}}_n]$  and apply Gaussian elimination to the augmented matrix (Section 2.3.2)  $[\tilde{\mathbf{B}}\tilde{\mathbf{B}}^\top | \tilde{\mathbf{B}}]$  to obtain an orthonormal basis. This constructive way to iteratively build an orthonormal basis  $\{\mathbf{b}_1, \dots, \mathbf{b}_n\}$  is called the *Gram-Schmidt process* (Strang, 2003).

#### Example 3.8 (Orthonormal Basis)

The canonical/standard basis for a Euclidean vector space  $\mathbb{R}^n$  is an orthonormal basis, where the inner product is the dot product of vectors.

In  $\mathbb{R}^2$ , the vectors

$$\mathbf{b}_1 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ 1 \end{bmatrix}, \quad \mathbf{b}_2 = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 \\ -1 \end{bmatrix} \quad (3.35)$$

form an orthonormal basis since  $\mathbf{b}_1^\top \mathbf{b}_2 = 0$  and  $\|\mathbf{b}_1\| = 1 = \|\mathbf{b}_2\|$ .

We will exploit the concept of an orthonormal basis in Chapter 12 and Chapter 10 when we discuss support vector machines and principal component analysis.

### 3.6 Orthogonal Complement

Having defined orthogonality, we will now look at vector spaces that are orthogonal to each other. This will play an important role in Chapter 10, when we discuss linear dimensionality reduction from a geometric perspective.

Consider a  $D$ -dimensional vector space  $V$  and an  $M$ -dimensional subspace  $U \subseteq V$ . Then its *orthogonal complement*  $U^\perp$  is a  $(D-M)$ -dimensional subspace of  $V$  and contains all vectors in  $V$  that are orthogonal to every vector in  $U$ . Furthermore,  $U \cap U^\perp = \{\mathbf{0}\}$  so that any vector  $\mathbf{x} \in V$  can be

orthogonal  
complement