

## MATHEMATICAL BACKGROUND

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We will assume that readers have basic knowledge of linear algebra and multivariable calculus. Since these skills may be a little rusty, however, here we recall an incomplete set of key ideas that will be used throughout our discussion. Readers comfortable with these topics can skip this chapter, although it is recommended they review especially the multivariable calculus sections and the discussion of Einstein notation.

### 2.1 LINEAR ALGEBRA

Although its simplicity and elegance place linear algebra in the pantheon of basic mathematical tools, linear algebra developed much later than geometry. While Euclid's *Elements* formalized aspects of geometry circa 300 BC, systematic study of linear problems did not take off until the seventeenth century [1]; that said, versions of basic linear algebra techniques such as Gaussian elimination appeared for millennia without being codified. At this point, however, we recognize linear algebra as a foundational tool both computationally and theoretically. Underscoring this point, the term “matrix” in linear algebra was invented in 1850 by J. Sylvester from the Latin word for *womb* [18].

#### 2.1.1 Basic Definitions

The main object of study in linear algebra is the *vector space*. For our purposes, rather than considering a general field  $F$ , we consider vector fields over the set of real numbers  $\mathbb{R}$ :

**Definition 2.1** (Vector space over  $\mathbb{R}$ ). *A vector space over  $\mathbb{R}$  is a set  $\mathbf{v}$  equipped with two binary operations  $+$  and  $\cdot$  satisfying the following axioms:*

- **GROUP AXIOMS:** For  $\mathbf{u}, \mathbf{v}, \mathbf{w} \in V$ , we have

$$\begin{aligned}\mathbf{u} + (\mathbf{v} + \mathbf{w}) &= (\mathbf{u} + \mathbf{v}) + \mathbf{w} && \text{(associativity)} \\ \mathbf{u} + \mathbf{v} &= \mathbf{v} + \mathbf{u} && \text{(commutativity)}.\end{aligned}$$

*In addition, there exists a zero element  $\mathbf{0} \in V$  such that  $\mathbf{v} + \mathbf{0} = \mathbf{v}$  for all  $\mathbf{v} \in V$ , and for each  $\mathbf{v} \in V$  there exists an additive inverse  $-\mathbf{v}$  such that  $\mathbf{v} + (-\mathbf{v}) = \mathbf{0}$ .*

- **VECTOR SPACE AXIOMS:** For  $a, b \in \mathbb{R}$  and  $\mathbf{u}, \mathbf{v} \in V$ , we have

$$\begin{aligned}a(\mathbf{u} + \mathbf{v}) &= a\mathbf{u} + a\mathbf{v} && \text{(distributivity)} \\ (a + b)\mathbf{v} &= a\mathbf{v} + b\mathbf{v} && \text{(distributivity)} \\ a(b\mathbf{v}) &= (ab)\mathbf{v} && \text{(associativity)} \\ 1\mathbf{v} &= \mathbf{v} && \text{(identity)}.\end{aligned}$$

*Our notation above drops the operator  $\cdot$  for multiplication. Elements of  $\mathbf{v}$  are called vectors; in this context we label real numbers in  $\mathbb{R}$  as scalars. A subset of a vector space that is itself a vector space is a subspace.*

Occasionally it will be useful to use complex rather than real numbers; the definition above suffices for that case, simply replacing  $\mathbb{R}$  with the set of complex numbers  $\mathbb{C} := \{a + b\sqrt{-1} : a, b \in \mathbb{R}\}$ .

From a high level, a vector space is any set of objects that can be (1) added together and (2) scaled. These two basic operations define a *linear combination*  $\mathbf{w} \in V$  of elements  $\{\mathbf{v}_k\}_{k=1}^m \subset V$  of a vector space  $\mathbf{v}$  with weights  $\{a^k\}_{k=1}^m$ :

$$\mathbf{w} = a^1 \mathbf{v}_1 + a^2 \mathbf{v}_2 + \cdots + a^m \mathbf{v}_m = \sum_{k=1}^m a^k \mathbf{v}_k.$$

To be clear, in this notation values like  $a^2$  represent the second element of  $a$ , rather than the squared value of a scalar  $a$ . See the aside in §2.1.3 for discussion of this notation.

The typical example of a vector space is Euclidean space  $\mathbb{R}^n$ , defined as the set of  $n$ -dimensional vectors. It is important to remember, however, that many other vector spaces exist that do not resemble Euclidean space. Two examples are below:

**Example 2.1** (Polynomials). *The set of polynomials of degree  $d$  is a vector space. Recall that a polynomial of degree  $d \in \mathbf{N}$  is any function  $\mathbf{p}(t)$  that can be written*

$$\mathbf{p}(t) = \sum_{k=0}^d a^k \mathbf{p}_k(t),$$

where the  $a^k$ 's are fixed constants and  $\mathbf{p}_k(t) := t^k$ . Adding two degree- $d$  polynomials together creates a third, as does scaling a polynomial by a constant:

$$\begin{aligned} \left( \sum_{k=0}^d a^k \mathbf{p}_k(t) \right) + \left( \sum_{k=0}^d b^k \mathbf{p}_k(t) \right) &= \sum_{k=0}^d (a^k + b^k) \mathbf{p}_k(t) \\ c \left( \sum_{k=0}^d a^k \mathbf{p}_k(t) \right) &= \sum_{k=0}^d (ca^k) \mathbf{p}_k(t). \end{aligned}$$

A straightforward exercise is to check that the axioms in Definition 2.1 hold for this set. In contrast, multiplying two degree- $d$  polynomials can make a degree- $2d$  polynomial, leaving the space; thankfully, Definition 2.1 only requires multiplication between scalars and vectors, not between two vectors.

**Example 2.2** ( $L^2$  functions). *The set  $L^2([0,1])$  is comprised of all functions  $f : [0,1] \rightarrow \mathbb{R}$  that are (Lebesgue) square-integrable:*

$$\int_0^1 f(t)^2 dt < \infty.$$

In particular, the integral must be defined and finite; in this case the axioms in Definition 2.1 reflect properties of the integral, e.g. that the integral of a sum of functions is the sum of their integrals.

The smallest subspace of a vector space  $\mathbf{v}$  containing a set of vectors  $\mathbf{v}_1, \dots, \mathbf{v}_m \in V$  is the *span*, defined by:

$$\text{span} \{ \mathbf{v}_1, \dots, \mathbf{v}_m \} := \left\{ v = \sum_{k=1}^m a^k \mathbf{v}_k : \{a^k\}_{k=1}^m \subset \mathbb{R} \right\}.$$

The span of a set of vectors can be thought of as the set of all vectors in  $\mathbf{v}$  “reachable” by linearly combining vectors in the set.

It could be the case that adding a new vector to a set does not change its span. For example, in  $\mathbb{R}^2$  we know  $\text{span} \{(1,0)\} = \text{span} \{(1,0), (2,0)\}$ . This is because  $(2,0) = 2 \cdot (1,0)$ , that is,  $(2,0)$  is already in the span of  $\{(1,0)\}$ . Hence, the latter case is somehow redundant. This idea is formalized in the definition of linear dependence:

**Definition 2.2** (Linear dependence). *A set of vectors  $W \subseteq V$  is linearly dependent if there exists a vector  $\mathbf{w} \in W$  that equals a linear combination of vectors in  $W \setminus \{\mathbf{w}\}$ . Otherwise the set is linearly independent.*

This leads to a key measure of the complexity of a vector space, its *dimension*:

**Definition 2.3** (Dimension). The dimension of a vector space  $\mathbf{v}$  is the maximum number of linearly independent vectors in any subset  $W \subseteq V$ .

**Example 2.3** (Standard basis for  $\mathbb{R}^n$ ). The dimension of Euclidean space  $\mathbb{R}^n$  is  $n$ , spanned by the standard basis vectors

$$\mathbf{e}_k := (\underbrace{0, \dots, 0}_{k-1 \text{ elements}}, 1, \underbrace{0, \dots, 0}_{n-k \text{ elements}}).$$

**Example 2.4.** Not all vector spaces have a finite dimension. For example, the space  $L^2([0, 1])$  from Example 2.2 is infinite-dimensional. While we know this intuitively (there are many functions!), one way to prove this is to show that the Fourier basis functions  $f_k(t) := \sin \pi k t$  are linearly independent for all  $k \in \mathbb{N}$ .

While we often illustrate vectors by drawing arrows, the reality of Definition 2.1 is that it is not particularly geometric. For example, it does not require there to be a notion of the length of a vector or the distance between two vectors. Formally, geometric structure is provided by *inner products*:

**Definition 2.4** (Inner product). An inner product on a vector space  $\mathbf{v}$  is a map  $g(\cdot, \cdot) : V \times V \rightarrow \mathbb{R}$  satisfying the following properties:

$$\begin{aligned} g(\mathbf{u}, \mathbf{v}) &= g(\mathbf{v}, \mathbf{u}) && \text{(symmetry)} \\ g(a\mathbf{u}, \mathbf{v}) &= ag(\mathbf{u}, \mathbf{v}) && \text{(linearity)} \\ g(\mathbf{u} + \mathbf{v}, \mathbf{w}) &= g(\mathbf{u}, \mathbf{w}) + g(\mathbf{v}, \mathbf{w}) && \text{(linearity)} \\ g(\mathbf{u}, \mathbf{u}) &\geq 0 \text{ with equality only when } \mathbf{u} = 0 && \text{(positive definiteness).} \end{aligned}$$

A key example of an inner product is the dot product  $\mathbf{v} \cdot \mathbf{w} := \mathbf{v}^\top \mathbf{w}$  on Euclidean space  $\mathbb{R}^n$ . A different example of an inner product is the following:

**Example 2.5** (Inner product of functions). Given  $f, g \in L^2([0, 1])$ , the  $L^2$  inner product  $\langle f, g \rangle$  is given by  $\langle f, g \rangle := \int_0^1 f(t)g(t) dt$ .

Inner products give a notion of length to a vector, via the definition of a *norm*:

$$\|\mathbf{v}\|_g := \sqrt{g(\mathbf{v}, \mathbf{v})}.$$

We will use the notation  $\|\mathbf{v}\|_2$  to denote the 2-norm of a vector from the dot product defined above.

Inner products also determine angles between vectors, motivated by the identity

$$\mathbf{v} \cdot \mathbf{w} = \|\mathbf{v}\|_2 \|\mathbf{w}\|_2 \cos \theta$$

in  $\mathbb{R}^3$  as well as the more general Cauchy–Schwarz inequality

$$|g(\mathbf{v}, \mathbf{w})| \leq \|\mathbf{v}\|_g \|\mathbf{w}\|_g,$$

which suggests that higher-dimensional inner products also have some notion of cosine between  $-1$  and  $1$ .

Using this idea to extend the idea of perpendicular vectors of dimension greater than three leads to the definition of *orthogonal* vectors  $v, w \in V$  as vectors satisfying  $g(\mathbf{v}, \mathbf{w}) = 0$ . An *orthonormal basis* is a basis of vectors  $\mathbf{v}_1, \mathbf{v}_2, \dots$  spanning a vector space  $\mathbf{v}$  such that

$$g(\mathbf{v}_k, \mathbf{v}_\ell) = \begin{cases} 1 & \text{if } k = \ell \\ 0 & \text{otherwise.} \end{cases}$$

### 2.1.2 Linear Maps

The power of linear algebra is in its characterization of *linear maps*, or maps from one vector space into another that preserve addition and scalar multiplication:

**Definition 2.5** (Linear map). *A map  $L[\cdot] : V \rightarrow W$  from vector space  $V$  into vector space  $W$  is linear if for any  $\mathbf{u}, \mathbf{v} \in V$  and  $c \in \mathbb{R}$  we have*

$$\begin{aligned} L[\mathbf{u} + \mathbf{v}] &= L[\mathbf{u}] + L[\mathbf{v}] & (\text{additivity}) \\ L[c\mathbf{u}] &= cL[\mathbf{u}] & (\text{linearity}). \end{aligned}$$

A corollary of this definition is that linear maps preserve the weights of linear combinations:

$$L\left[\sum_{k=1}^p a^k \mathbf{v}_k\right] = \sum_{k=1}^p a^k L[\mathbf{v}_k],$$

for any collection of vectors  $\mathbf{v}_1, \dots, \mathbf{v}_p \in V$  and scalars  $a^1, \dots, a^p \in \mathbb{R}$ . Linear maps also necessarily take the zero element of one vector space to the zero element of another.

The best-known linear operators are given as matrix-vector products, explored in §2.1.3, but others exist. One example is as follows:

**Example 2.6** (Linear operator). *Consider the following operator from  $L^2([0, 1])$  into  $\mathbb{R}$ :*

$$L[f] := \int_0^1 f(t) dt.$$

*This map takes elements of one vector space, functions in  $L^2([0, 1])$ , and maps them to elements of another vector space, scalars in  $\mathbb{R}^1$ . Checking that  $L$  is linear involves two tests:*

$$\begin{aligned} L[f + g] &= \int_0^1 [f(t) + g(t)] dt = \int_0^1 f(t) dt + \int_0^1 g(t) dt = L[f] + L[g] \\ L[cf] &= \int_0^1 cf(t) dt = c \int_0^1 f(t) dt = cL[f]. \end{aligned}$$

The *kernel* or *null space* of a linear operator  $L : V \rightarrow W$  is the set of vectors  $L$  maps to the zero element of  $\mathbf{w}$ :

$$\text{kernel } L := \{\mathbf{v} \in V : L[\mathbf{v}] = 0\}.$$

The *image* of  $L$  is the subspace of  $\mathbf{w}$  corresponding to vectors mapped under  $L$ :

$$\text{image } L := \{\mathbf{w} \in W : \mathbf{w} = L[\mathbf{v}] \text{ for some } \mathbf{v} \in V\}.$$

In the finite-dimensional case, the image is also known as the *column space*, since it is the span of the columns of  $L$  represented as a matrix; the dimension of the column space is known as the *rank*.

### 2.1.3 Euclidean Space

Our discussion above has been generic to any vector space over the real numbers, but most computational applications of linear algebra involve a single vector space, Euclidean space  $\mathbb{R}^n$ .

A vector in  $\mathbb{R}^n$  can be represented using a tuple of values  $\mathbf{v} = (v^1, v^2, \dots, v^n)$ , which serves as a compact way of writing  $\mathbf{v}$  in the standard basis introduced in Example 2.3:

$$\mathbf{v} = \sum_{k=1}^n v^k \mathbf{e}_k.$$

A third more space-consuming option that aligns well with calculations in linear algebra is to write  $\mathbf{v}$  as an  $n \times 1$  column:

$$\mathbf{v} = \begin{pmatrix} v^1 \\ v^2 \\ \vdots \\ v^n \end{pmatrix}. \quad (2.1)$$

All of these coordinate-wise representations in terms of  $v^1, \dots, v^n$  implicitly involve the standard basis vectors  $\mathbf{e}_i$ , which is of course not the only basis for  $\mathbb{R}^n$ .

**Aside** (Einstein notation). *Note our usage of upper indices  $v^k$  for the coefficients of  $\mathbf{v}$  in the standard basis, notated with lower indices  $\mathbf{e}_k$ . This choice is not by accident but rather suggestive of a convention in differential geometry known as Einstein notation, in which any time an index is repeated twice (once upper, once lower) it is implicitly summed. For instance, we could write:*

$$\mathbf{v} = v^k \mathbf{e}_k.$$

*This notation can be confusing to readers who do not work with it every day, so with the possible exception of a few tedious calculations we will avoid dropping summation operators.*

Suppose  $L : \mathbb{R}^n \rightarrow \mathbb{R}^m$  is a linear map. Applying the basic properties of linearity, for any vector  $\mathbf{v} \in \mathbb{R}^n$  we have

$$L[\mathbf{v}] = L \left[ \sum_{k=1}^n v^k \mathbf{e}_k \right] = \sum_{k=1}^n v^k L[\mathbf{e}_k].$$

In other words, the map  $L$  is *completely determined* by its action on the standard basis vectors  $\mathbf{e}_1, \mathbf{e}_2, \dots, \mathbf{e}_n$ . This suggests representing  $L$  using a *matrix*

$$L \sim \begin{pmatrix} | & | & \cdots & | \\ L[\mathbf{e}_1] & L[\mathbf{e}_2] & \cdots & L[\mathbf{e}_n] \\ | & | & \cdots & | \end{pmatrix} \in \mathbb{R}^{m \times n}.$$

We repeat here that this representation of  $L$  is *in the standard basis*, which may not be canonical for a problem that is rotated from the  $xyz$  axes.

There are many advantages of the matrix representation for  $L$ . In particular, it makes sense computationally to store a grid of numbers, and a vector is a special case of a matrix with a single column, as in (2.1). In addition, matrix-vector multiplication (and matrix-matrix multiplication as a generalization) admits a simple mnemonic, moving from left to right in the first term and top to bottom in the second:

$$L[\mathbf{v}] = \begin{pmatrix} | & | & \cdots & | \\ L[\mathbf{e}_1] & L[\mathbf{e}_2] & \cdots & L[\mathbf{e}_n] \\ | & | & \cdots & | \end{pmatrix} \begin{pmatrix} v^1 \\ v^2 \\ \vdots \\ v^n \end{pmatrix} \rightarrow \sum_{k=1}^n v^k L[\mathbf{e}_k].$$

For consistency with our (admittedly pedantic) choice of index notation, when a matrix represents a linear map we will use one upper index and one lower index to represent its individual elements in the standard basis:

$$\begin{pmatrix} L_1^1 & L_2^1 & \cdots & L_n^1 \\ L_1^2 & L_2^2 & \cdots & L_n^2 \\ \vdots & \vdots & \ddots & \vdots \\ L_1^m & L_2^m & \cdots & L_n^m \end{pmatrix} \begin{pmatrix} v^1 \\ v^2 \\ \vdots \\ v^n \end{pmatrix} = \begin{pmatrix} \sum_{k=1}^n L_k^1 v^k \\ \sum_{k=1}^n L_k^2 v^k \\ \vdots \\ \sum_{k=1}^n L_k^m v^k \end{pmatrix} := \begin{pmatrix} w^1 \\ w^2 \\ \vdots \\ w^m \end{pmatrix}. \quad (2.2)$$

Here,  $L_j^i$  is the coefficient of  $L[\mathbf{e}_j]$  in the  $\mathbf{e}_i$  direction:  $L_j^i = \mathbf{e}_i \cdot L[\mathbf{e}_j]$ . Notice this notation is somewhat misleading when  $m \neq n$ :  $\mathbf{e}_i \in \mathbb{R}^m$  and  $\mathbf{e}_j \in \mathbb{R}^n$ , so they are technically standard basis vectors in different dimensions.

Matrices also appear when considering inner products between vectors; we will distinguish this case by changing the positions of the indices. Suppose  $g(\cdot, \cdot)$  is an inner product on  $\mathbb{R}^n$ . By bilinearity, we can write:

$$g(\mathbf{v}, \mathbf{w}) = g\left(\sum_{k=1}^n v^k \mathbf{e}_k, \sum_{\ell=1}^n w^\ell \mathbf{e}_\ell\right) = \sum_{k,\ell=1}^n v^k w^\ell g(\mathbf{e}_k, \mathbf{e}_\ell). \quad (2.3)$$

Hence, if we notate  $g_{k\ell} := g(\mathbf{e}_k, \mathbf{e}_\ell)$  then in Einstein notation we have  $g(\mathbf{v}, \mathbf{w}) = v^k w^\ell g_{k\ell}$ .

We can also store the values  $g_{k\ell}$  in a matrix, but the entries of the matrix have a different meaning: They are inner products of the standard basis vectors instead of images of the standard basis vectors under a linear map. This distinction explains our different choice of index positions. This aside, if we define  $G \in \mathbb{R}^{n \times n}$  as a matrix with entries  $g_{k\ell}$ , we have

$$g(\mathbf{v}, \mathbf{w}) = \sum_{k,\ell=1}^n g_{k\ell} v^k w^\ell = \mathbf{v}^\top G \mathbf{w},$$

where we think of  $\mathbf{v}$  and  $\mathbf{w}$  as  $n \times 1$  matrices and the result of the product is a  $1 \times 1$  matrix, or scalar. Here,  $\top$  denotes the *transpose* operator, which flips the two indices of a matrix.

**Example 2.7** (Dot product). Recall that the “dot product” of two vectors  $v, w \in \mathbb{R}^n$  is defined as

$$\mathbf{v} \cdot \mathbf{w} := \mathbf{v}^\top \mathbf{w}.$$

From our discussion above, it is evident that the dot product is an inner product with the choice  $G = I_{n \times n}$ , the identity matrix. In other words, the implicit assumption in computing a dot product is that the inner product of two standard basis vectors is given by

$$\mathbf{e}_i \cdot \mathbf{e}_j = \delta_{ij} := \begin{cases} 1 & \text{if } i = j \\ 0 & \text{otherwise.} \end{cases}$$

Unless otherwise noted, we will assume  $\mathbb{R}^n$  is equipped with the dot product as its inner product.

#### 2.1.4 Linear Systems of Equations

Countless contexts in linear algebra—and nearly any other branch of mathematics—require the solution of *inverse problems*, in which we attempt to undo the action of some mathematical operator. A counterintuitive theme is that solving a *forward problem* and finding its inverse require different machinery. For example, multiplying a set of prime numbers to find a product is easy even when the product is a fairly large number, while finding the prime factors of a large integer can take tons of computational time. While inverting a linear map is not nearly as challenging as prime factorization, the inversion of a linear map  $L$  is a formidable algorithmic task to carry out efficiently and stably.

Given a linear map from  $\mathbb{R}^n$  to  $\mathbb{R}^m$  represented as a matrix  $A \in \mathbb{R}^{m \times n}$  and a vector  $\mathbf{b} \in \mathbb{R}^m$ , the basic linear system equations asks to find  $\mathbf{x} \in \mathbb{R}^n$  such that  $A\mathbf{x} = \mathbf{b}$ . This problem is solvable any time  $\mathbf{b}$  is in the column space of  $A$  (regardless of  $m$  and  $n$ !).

Basic algorithms for solving  $A\mathbf{x} = \mathbf{b}$  often assume  $A$  is *invertible*, meaning one can find exactly one  $\mathbf{x}$  corresponding to any  $\mathbf{b}$ . The linear map  $\mathbf{x} \mapsto A\mathbf{x}$  certainly must be bijective for  $A$  to be invertible, so by dimension-counting we must have  $m = n$  in this case. Accompanying the condition that  $A$  is square, several equivalent conditions imply invertibility of  $A$ :

- The columns (or rows) of  $A$  span  $\mathbb{R}^n$ .

- The columns (or rows) of  $A$  are linearly independent.
- $A\mathbf{x} = \mathbf{0}$  implies  $\mathbf{x} = \mathbf{0}$ .
- The determinant of  $A$  is nonzero.

In any of these cases,  $A$  admits an inverse matrix  $A^{-1}$  so that  $AA^{-1} = A^{-1}A = I_{n \times n}$ .

A considerable portion of introductory linear algebra coursework is dedicated to solving  $A\mathbf{x} = \mathbf{b}$  by hand, but the reality is that there exist relatively stable and efficient algorithms and software for doing this in practice. Typical algorithms include Gaussian elimination, LU factorization, and iterative methods like conjugate gradients (CG). In our discussion, we will assume that a “black box” implementation of a linear solver is at our disposal, so we do not need to discuss these algorithms in detail; see [CITE] for detailed discussion.

One notable algorithmic consideration for solving linear systems is the identification of *structure* in the matrix  $A$ . If we know more information about the contents of  $A$ , we may be able to choose more efficient algorithms than the sledgehammer techniques used to invert any  $A \in \mathbb{R}^{n \times n}$ . Properties that can be leveraged include the following:

- *Positive definite* matrices  $A$  (notated  $A \succeq 0$ ) satisfy the property  $\mathbf{x}^\top A \mathbf{x} \geq 0$  for any  $\mathbf{x} \in \mathbb{R}^n$  with  $\mathbf{x}^\top A \mathbf{x} = 0$  if and only if  $\mathbf{x} = \mathbf{0}$ ; the latter condition is relaxed for *positive semidefinite* matrices. In this case, we can always factor  $A = LL^\top$  where  $L$  is lower-triangular, using the Cholesky factorization. Then,  $A^{-1} = L^{-\top}L^{-1}$ , where the inverse of  $L$  and its transpose are algorithmically easier to compute.
- The entries of *sparse* matrices are mostly zero. This is by far the most common scenario in low-dimensional geometry processing and in graph theory, since often each row/column of a matrix corresponds to a single vertex on a mesh with nonzeros only when vertices share an edge. Sparse matrices might be stored using a long list of triplets (row, column, value) rather than as an  $m \times n$  grid of mostly zero values. Specialized algorithms factor and invert sparse matrices in time proportional to the number of nonzero elements rather than  $mn$ .
- *Structured* matrices might have repeated blocks, which may be easier to store once rather than copying the blocks multiple times.
- Some matrices are easy to apply but hard to write explicitly. For instance, for fixed matrices  $A, B \in \mathbb{R}^{n \times n}$  the following is a linear operator:

$$f(C) = CA + AC.$$

We could try to recover  $C$  from  $f(C)$  by writing  $C$  as a long vector in  $\mathbb{R}^{n^2}$  and then figuring out the corresponding  $n^2 \times n^2$  matrix representing the action of  $f$ , but this calculation is tedious and inefficient. Instead, it may be easier to provide a piece of code that implements the linear map  $C \mapsto f(C)$  without giving the elements of the corresponding matrix explicitly, in which case iterative algorithms like gradient descent and conjugate gradients can be preferable for inverting  $f$ .

The guide above is vague in the sense that we do not provide algorithmic details. This is on purpose: It is rare to need to implement a numerical linear algebra algorithm in practice, since well-tested implementations are available for free. Languages such as Python and Matlab have these built-in, and libraries such as Eigen [CITE] and SuiteSparse [CITE] provide implementations in languages like C++.

**Warning.** *There is rarely a need to compute  $A^{-1}$  from  $A \in \mathbb{R}^{n \times n}$  explicitly. Many algorithms can solve the system  $A\mathbf{x} = \mathbf{b}$  from a single  $\mathbf{b}$  much faster than computing all of  $A^{-1}$  and then multiplying to obtain  $\mathbf{x} = A^{-1}\mathbf{b}$ . Furthermore, inverting matrices explicitly can ruin their structure; for instance, the inverse of a sparse matrix is rarely sparse.*

**Example 2.8** (Least-squares). Suppose we wish to solve the following least-squares problem for  $\mathbf{x} \in \mathbb{R}^n$  given  $A \in \mathbb{R}^{m \times n}$  and  $\mathbf{b} \in \mathbb{R}^m$ :

$$\min_{\mathbf{x} \in \mathbb{R}^n} \|A\mathbf{x} - \mathbf{b}\|_2^2. \quad (2.4)$$

Intuition for this problem is illustrated in Figure [REF](#). This problem appears when we are not confident if  $\mathbf{b}$  is in the column space of  $A$ , and hence we want to find the  $\mathbf{x}$  for which  $A\mathbf{x}$  is as close as possible to  $\mathbf{b}$ . Using the techniques e.g. in §2.2.2, we can show that the optimal  $\mathbf{x}$  satisfies the normal equations

$$A^\top A\mathbf{x} = A^\top \mathbf{b}. \quad (2.5)$$

We can check that  $A^\top A$  is positive semidefinite:

$$\mathbf{x}^\top A^\top A\mathbf{x} = (A\mathbf{x})^\top (A\mathbf{x}) = \|A\mathbf{x}\|_2^2 \geq 0.$$

The matrix  $A^\top A$  is invertible when  $A$  has linearly independent columns. If  $A$  is square then in this case  $A$  is invertible. If  $A$  is non-square but has linearly independent columns, the least-squares problem is over-determined but still (2.5) determines a unique solution for (2.4). When the columns of  $A$  are linearly dependent,  $A^\top A$  is not invertible, indicating (2.4) has a nonunique solution.

### 2.1.5 Eigenproblems

The last linear algebra problem we consider is the *eigenvector* problem:

**Definition 2.6** (Eigenvector). An eigenvector of a linear transformation  $L : V \rightarrow V$  acting on vector space  $V$  is a vector  $\mathbf{v} \in V \setminus \{\mathbf{0}\}$  such that

$$L[\mathbf{v}] = \lambda \mathbf{v} \quad (2.6)$$

for some  $\lambda \in \mathbb{R}$ . In this case,  $\lambda$  is known as the *eigenvalue* corresponding to eigenvector  $\mathbf{v}$ .

As illustrated in Figure [REF](#), geometrically eigenvectors are directions in which the linear transformation  $L$  scales a vector without rotating it.

**Example 2.9** (Eigenvector of a matrix). The eigenvectors of the matrix

$$M := \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$$

are given by

$$\mathbf{v}_1 = \begin{pmatrix} -1 \\ 1 \end{pmatrix} \quad \text{and} \quad \mathbf{v}_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}.$$

In particular,

$$\begin{aligned} M\mathbf{v}_1 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} -1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix} = -1 \cdot \mathbf{v}_1 \\ M\mathbf{v}_2 &= \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix} = 1 \cdot \mathbf{v}_2. \end{aligned}$$

The corresponding eigenvalues of  $M$  are  $\lambda_1 = -1$  and  $\lambda_2 = 1$ .

Example 2.9 illustrates a slight abuse of language typical in the linear algebra world. Here, “the eigenvectors” of  $M$  include not only  $\mathbf{v}_1$  and  $\mathbf{v}_2$  but also these two vectors scaled by any nonzero real number.



**Example 2.10** (Eigenfunctions). Take  $C^\infty([0, 1])$  to be the set of differentiable functions  $f : [0, 1] \rightarrow \mathbb{R}$ . Define the operator  $L : C^\infty([0, 1]) \rightarrow C^\infty([0, 1])$  given by the second derivative

$$L[f] = f''.$$

For instance,

$$L[t^2] = \frac{d^2}{dt^2} t^2 = 2 \quad \text{and} \quad L[\log(t+1)] = \frac{d^2}{dt^2} \log(t+1) = -\frac{1}{(t+1)^2}.$$

Then, eigenfunctions of  $L$  include  $e^{at}$  and  $\cos at$ , since

$$L[e^{at}] = a^2 \cdot e^{at} \quad \text{and} \quad L[\cos at] = -a^2 \cdot \cos at.$$

The corresponding eigenvalues are  $a^2$  and  $-a^2$ .

We conclude our discussion of classic linear algebra by quoting a famous theorem regarding the eigenvectors of a symmetric matrix:

**Theorem 2.1** (Spectral theorem). If  $A \in \mathbb{R}^{n \times n}$  is symmetric, there exists an orthonormal basis for  $\mathbb{R}^n$  (with respect to the dot product  $\mathbf{v} \cdot \mathbf{w} = \mathbf{v}^\top \mathbf{w}$ ) of eigenvectors of  $A$ .

## 2.2 MULTIVARIABLE CALCULUS

To consider *curved* rather than flat geometry, we need multivariable tools that extend beyond the reach of linear algebra. That is, most spaces are nonlinear—although we may approximate them locally with linear objects. Multivariable calculus equips us with the machinery we need to understand maps in the more general case.

### 2.2.1 Optimization

A key motivator for differential calculus is to study *optimization* problems. In one variable, the connection between optimization and calculus is derived by noticing that minimizing a function  $f(x) : \mathbb{R} \rightarrow \mathbb{R}$  is equivalent—under a differentiability assumption—to finding roots of the first derivative  $f'(x)$ ; the sign of the second derivative  $f''(x)$  then determines whether critical points  $x \in \mathbb{R}$  satisfying  $f'(x) = 0$  are minima, maxima, or indeterminate. We follow a similar path here for functions on  $\mathbb{R}^n$  to define the gradient and Hessian.

### 2.2.2 Gradients and Hessians

Suppose  $f(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$  is a function<sup>1</sup> that assigns a real value to every point in  $\mathbb{R}^n$ . In analogy to one-dimensional optimization problems, we might wish to find an  $\mathbf{x} \in \mathbb{R}^n$  that achieves the minimum value of  $f$  locally or globally.

As illustrated in Figure [REF](#), if a point  $\mathbf{x}_0 \in \mathbb{R}^n$  is a local minimum of  $f$ , then in particular it locally minimizes  $f$  along any one-dimensional slice through  $\mathbf{x}_0$ . Formalizing this idea, take an arbitrary  $\mathbf{v} \in \mathbb{R}^n$  and define the *differential* of  $f$  at  $\mathbf{x}_0$  as

$$df_{\mathbf{x}_0}(\mathbf{v}) := \lim_{h \rightarrow 0} \frac{f(\mathbf{x}_0 + h\mathbf{v}) - f(\mathbf{x}_0)}{h}.$$

As a motivator for proofs we will do in differential geometry, we note the following property:

**Proposition 2.1.**  $df_{\mathbf{x}_0} : \mathbb{R}^n \rightarrow \mathbb{R}$  is a linear operator.

<sup>1</sup> Here and in our subsequent discussion, we will ignore (important) considerations regarding differentiability and instead will assume all functions are smooth.

*Proof.* Applying one-dimensional calculus  $n$  times shows

$$f(\mathbf{x}_0 + h\mathbf{v}) = f(\mathbf{x}_0) + h \sum_{k=1}^n \frac{\partial f}{\partial x_k} v^k + O(h^2), \quad (2.7)$$

where we expand  $v = \sum_k v^k \mathbf{e}_k$ . Here,  $\frac{\partial f}{\partial x_k}$  denotes the  $k$ -th *partial derivative*, or derivative of  $f$  considered as a one-variable function along coordinate  $k$ . Plugging this expansion into the definition of  $df_{\mathbf{x}_0}$  yields the desired result.  $\square$

While the previous proposition does not require *any* inner product on  $\mathbb{R}^n$  to make sense, a closer examination of (2.7) (or application of exercise 2.4.) shows existence of a vector  $\nabla f(\mathbf{x}_0) \in \mathbb{R}^n$  so that

$$df_{\mathbf{x}_0}(\mathbf{v}) = \nabla f(\mathbf{x}_0) \cdot \mathbf{v}.$$

Note the *direction* of  $\nabla f$  might change if we equip  $\mathbb{R}^n$  with a different inner product; see exercise 2.4. for details.

In any event, we define a *critical point* of a function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  to be any  $\mathbf{x}_0 \in \mathbb{R}^n$  satisfying  $df_{\mathbf{x}_0} \equiv 0$ , or equivalently  $\nabla f(\mathbf{x}_0) = \mathbf{0}$ . If  $f$  is differentiable, any local minimum or maximum of  $f$  is a critical point. If we wish to minimize  $f$ , after finding its critical points we have to verify which of the critical points are local minima. Continuing to apply the logic of Figure [REF](#),  $\mathbf{x}_0 \in \mathbb{R}^n$  is a local minimum of  $f$  only if it is a local minimum along any line through  $\mathbf{x}_0$ .

A similar argument to that of Proposition 2.1 shows existence of a *bilinear* operator  $H_{\mathbf{x}_0}(\mathbf{v}, \mathbf{w})$  such that  $H_{\mathbf{x}_0}(\mathbf{v}, \mathbf{v}) = \frac{d^2}{dh^2} f(\mathbf{x}_0 + h\mathbf{v})$ ; in Euclidean coordinates this justifies the Taylor expansion

$$f(\mathbf{x}_0 + \mathbf{v}) = f(\mathbf{x}_0) + \mathbf{v} \cdot \nabla f(\mathbf{x}_0) + \frac{1}{2} \mathbf{v}^\top H_{\mathbf{x}_0} \mathbf{v} + O(\|\mathbf{v}\|_2^2),$$

where  $H_{\mathbf{x}_0}$  in this context is the *Hessian matrix* of second partial derivatives of  $f$ ; when  $H_{\mathbf{x}_0}$  is positive definite at a critical point  $\mathbf{x}_0$ , we know  $\mathbf{x}_0$  is a local minimum of  $f$ .

**Example 2.11** (Least-squares). Suppose we wish to minimize the function

$$f(\mathbf{x}) = \frac{1}{2} \|A\mathbf{x} - \mathbf{b}\|_2^2,$$

where  $A \in \mathbb{R}^{m \times n}$  and  $\mathbf{b} \in \mathbb{R}^m$ . The gradient of  $f$  is

$$\nabla_{\mathbf{x}} f(\mathbf{x}) = A^\top A\mathbf{x} - A^\top \mathbf{b}.$$

Setting this expression to zero verifies the famous normal equations

$$A^\top A\mathbf{x} = A^\top \mathbf{b}$$

characterizing the solution to least-squares problems. The Hessian of  $f$  has no dependence on  $\mathbf{x}$ :

$$H \equiv A^\top A.$$

$A^\top A$  is positive definite when  $A$  has full column rank, verifying that  $\mathbf{x} = (A^\top A)^{-1} A^\top \mathbf{b}$  is the unique global minimizer of the least-squares problem in this case.

### 2.2.3 Lagrange Multipliers and KKT Conditions

A unique aspect of multivariable calculus is that it is possible to add *constraints* to an optimization problem. That is, rather than minimizing a function  $f(\mathbf{x})$  over all possible  $\mathbf{x} \in \mathbb{R}^n$ , we might restrict to a subset of admissible  $\mathbf{x}$  values to some subset:  $\mathbf{x} \in S \subseteq \mathbb{R}^n$ ; a point satisfying the constraint is called *feasible*. While constraints are easy to deal with when  $n = 1$  since they typically just specify

a range of  $\mathbf{x}$  values, e.g.  $x \in [a, b]$ , as shown in Figure [REF](#) higher-dimensional constraints might specify curves or regions.

Suppose in addition to our objective function  $f(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}$  we are given a second function  $g(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^m$ . As illustrated in Figure [REF](#), we could ask to find the minimum of a function  $f(\mathbf{x})$  subject to the constraint that  $\mathbf{x}$  is in the *zero level set*  $\{\mathbf{x} : g(\mathbf{x}) = \mathbf{0}\}$ :

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^n} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & g(\mathbf{x}) = \mathbf{0}. \end{aligned} \tag{2.8}$$

The function  $g(\mathbf{x})$  takes values in  $\mathbb{R}^m$ , implicitly encoding  $m$  potentially independent constraints  $g_1(\mathbf{x}) = 0, \dots, g_m(\mathbf{x}) = 0$ .

Our goal is to derive first-order conditions for local optima for the constrained problem, similar to  $\nabla f = \mathbf{0}$  in the unconstrained case. To give intuition for these conditions, we take the coarsest possible approximation of  $f$  and the components of  $g$ :

$$\begin{aligned} f(\mathbf{x}_0 + \mathbf{v}) &= f(\mathbf{x}_0) + \nabla f(\mathbf{x}_0)^\top \mathbf{v} + O(\|\mathbf{v}\|_2^2) \\ g_k(\mathbf{x}_0 + \mathbf{v}) &= g_k(\mathbf{x}_0) + \nabla g_k(\mathbf{x}_0)^\top \mathbf{v} + O(\|\mathbf{v}\|_2^2) \quad \forall k \in \{1, \dots, m\}. \end{aligned}$$

Suppose  $\mathbf{x}_0$  satisfies the constraints:  $g(\mathbf{x}_0) = \mathbf{0}$ . By the expressions above, a small perturbation  $\mathbf{v}$  of  $\mathbf{x}_0$  maintaining the constraint must satisfy  $\nabla g_k(\mathbf{x}_0)^\top \mathbf{v} = 0$  for all  $k$ . In other words, we need  $\mathbf{v}$  to be orthogonal to the span of the  $\nabla g_k(\mathbf{x}_0)$ 's:

$$\mathbf{v} \perp \text{span} \{ \nabla g_k(\mathbf{x}_0) : k \in \{1, \dots, m\} \} = \left\{ \sum_k \lambda^k \nabla g_k(\mathbf{x}_0) : \lambda_1, \dots, \lambda_m \in \mathbb{R} \right\}.$$

On the other hand, a perturbation  $\mathbf{v}$  to (strictly) decrease from  $f(\mathbf{x}_0)$  to  $f(\mathbf{x}_0 + \mathbf{v})$  must satisfy  $\nabla f(\mathbf{x}_0)^\top \mathbf{v} \neq 0$ .

Putting these arguments together, a local optimum  $\mathbf{x}_0$  of  $f$  subject to  $g = \mathbf{0}$  has the property that *any* small perturbation  $\mathbf{v}$  of  $\mathbf{x}_0$  that decrease  $f$  must violate the constraints. In symbols, there exist  $\lambda^1, \dots, \lambda^m$  such that

$$\nabla f(\mathbf{x}_0) = - \sum_{k=1}^m \lambda^k \nabla g_k(\mathbf{x}_0). \tag{2.9}$$

The sign on the right-hand side is arbitrary and chosen for a convention we will establish below. The coefficients  $\lambda^k$  are known as *Lagrange multipliers* or *dual variables*, providing a first-order optimality condition for equality-constrained optimization. Intuition for this condition is illustrated in Figure [REF](#).

If we define the *Lagrangian function*

$$\Lambda(\mathbf{x}; \lambda) := f(\mathbf{x}) + \sum_{k=1}^m \lambda^k g_k(\mathbf{x}),$$

then it is easy to check that the Lagrange multiplier condition (2.9) is equivalent to finding a critical point of  $\Lambda$  with respect to both  $\mathbf{x} \in \mathbb{R}^n$  and  $\lambda \in \mathbb{R}^m$  simultaneously. One tricky aspect of this observation is explored in problem 2.5.: Solutions of the constrained optimization problem (2.8) are minima with respect to  $\mathbf{x}$  and maxima with respect to  $\lambda$ .

**Example 2.12** (Eigenvalue problems). For symmetric, positive definite  $A \in \mathbb{R}^{n \times n}$ , consider the optimization problem

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^n} \quad & \mathbf{x}^\top A \mathbf{x} \\ \text{subject to} \quad & \|\mathbf{x}\|_2^2 = 1. \end{aligned}$$

This problem has Lagrangian

$$\Lambda(\mathbf{x}; \lambda) = \mathbf{x}^\top A \mathbf{x} + \lambda(1 - \|\mathbf{x}\|_2^2).$$

Setting the derivative with respect to  $\mathbf{x}$  to zero shows

$$A\mathbf{x} = \lambda\mathbf{x}.$$

This gives an optimization-oriented interpretation of the smallest eigenvector of a positive definite matrix, as the minimizer of  $\mathbf{x}^\top A\mathbf{x}$  with a unit norm constraint; note without the constraint the minimizer would simply be  $\mathbf{x} = \mathbf{0}$ .

As illustrated in Figure [REF](#), a more general constraint can be expressed as  $h(\mathbf{x}) \leq \mathbf{0}$ , where  $h(\mathbf{x}) : \mathbb{R}^n \rightarrow \mathbb{R}^p$ ; here, we use the convention that  $h(\mathbf{x}) \leq \mathbf{0} \iff h_1(\mathbf{x}) \leq 0, \dots, h_p(\mathbf{x}) \leq 0$ . This is a generalization of the equality constraints discussed above, since  $h(\mathbf{x}) \leq \mathbf{0}$  and  $-h(\mathbf{x}) \leq \mathbf{0}$  together imply  $h(\mathbf{x}) = \mathbf{0}$ .

Suppose  $\mathbf{x}_0 \in \mathbb{R}^n$  is a local optimum for the problem

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^n} \quad & f(\mathbf{x}) \\ \text{subject to} \quad & h(\mathbf{x}) \leq \mathbf{0}. \end{aligned} \tag{2.10}$$

Then, for each component  $h_k$ ,  $k \in \{1, \dots, p\}$ , we have two possibilities:

- $h_k$  is *active* at  $\mathbf{x}_0$  if  $h_k(\mathbf{x}_0) = 0$ . Typically (although not always!), if a constraint is active it implies that removing the constraint from the optimization problem would affect the position of the optimal  $\mathbf{x}_0$ . In other words, minimizing  $f$  without constraint  $k$  would result in an even lower value of  $f$ . Conversely, if we changed constraint  $k$  from an inequality constraint to an equality constraint, we would not expect the solution to change.
- $h_k$  is *inactive* at  $\mathbf{x}_0$  if  $h_k(\mathbf{x}_0) < 0$  strictly. In this case, assuming  $h_k$  is continuous we know that  $h_k(\mathbf{x}) < 0$  in some neighborhood of  $\mathbf{x}_0$ , so removing constraint  $k$  would not locally affect the position of the local minimum  $\mathbf{x}_0$ .

We can extend Lagrange multipliers to this case. By the logic above, we could throw away all inactive constraints at a critical point  $\mathbf{x}_0$  and convert active inequality constraints to equality constraints  $h_k(\mathbf{x}_0) = 0$ . Define  $\lambda^k$  to be either 0 if a constraint is inactive or to be the Lagrange multiplier for the equality-constrained problem at a critical point. We can write this definition compactly via the “complementary slackness” constraint:

$$0 = \lambda^k h_k(\mathbf{x}_0) \quad \forall k \in \{1, \dots, p\}.^2 \tag{2.11}$$

This constraint on  $\lambda^k$  forces it to be zero if  $g_k$  is nonzero. Additionally, since we zeroed out irrelevant terms we still have the “stationarity condition”

$$0 = \nabla f(\mathbf{x}_0) + \sum_{k=1}^p \lambda^k \nabla h_k(\mathbf{x}_0). \tag{2.12}$$

It is acceptable if we perturb  $\mathbf{x}_0$  in a direction that converts an active constraint into an inactive one, that is, if we move to the *interior* of constraint  $k$ . From (2.9), we can think of the nonzero  $\lambda^k$ s as the components of  $-\nabla f(\mathbf{x}_0)$  in the  $\nabla h_k(\mathbf{x}_0)$  basis. Recalling that  $-\nabla f(\mathbf{x}_0)$  is the first-order *descent* direction for  $f$ , we can enforce that any perturbation that decreases  $f$  will violate an active constraint via the *dual feasibility* constraint

$$\lambda^k \geq 0. \tag{2.13}$$

In total, conditions (2.11)–(2.13) together with the “primal feasibility” constraint  $h(\mathbf{x}_0) \leq \mathbf{0}$  form the Karush–Kuhn–Tucker (KKT) conditions for inequality-constrained optimization.

<sup>2</sup> This is *not* Einstein notation: This product is zero for each  $k$  independently.

**Example 2.13** (Nonnegative projection). Suppose we wish to find the closest vector  $\mathbf{x} \in \mathbb{R}^n$  to a vector  $\mathbf{x}_0 \in \mathbb{R}^n$  with only nonnegative elements. We can express this as an optimization problem:

$$\begin{aligned} \min_{\mathbf{x} \in \mathbb{R}^n} \quad & \|\mathbf{x} - \mathbf{x}_0\|_2^2 \\ \text{subject to} \quad & \mathbf{x} \geq 0. \end{aligned}$$

In this case, we can write  $h_k(\mathbf{x}) = -\mathbf{x} \cdot \mathbf{e}_k$ , the  $k$ -th component of the vector  $\mathbf{x}$ . In this case, the KKT conditions are as follows

$$\begin{aligned} \text{Complementary slackness:} \quad & \lambda^k(\mathbf{x} \cdot \mathbf{e}_k) = 0 \\ \text{Stationarity:} \quad & 2(\mathbf{x} - \mathbf{x}_0) - \sum_{k=1}^n \lambda^k \mathbf{e}_k = 0 \\ \text{Dual feasibility:} \quad & \lambda^1, \dots, \lambda^n \geq 0 \\ \text{Primal feasibility:} \quad & \mathbf{x} \cdot \mathbf{e}_1, \dots, \mathbf{x} \cdot \mathbf{e}_n \geq 0. \end{aligned}$$

Taking dot products on both sides of the stationarity condition shows

$$2\mathbf{e}_k \cdot (\mathbf{x} - \mathbf{x}_0) = \lambda^k.$$

We have two cases:

1. If  $\lambda^k = 0$ , we know  $\mathbf{x} \cdot \mathbf{e}_k = \mathbf{x}_0 \cdot \mathbf{e}_k$ , in other words, the  $k$ -th entry in  $\mathbf{x}$  is identical to that of  $\mathbf{x}_0$ . By primal feasibility, this can only happen when  $\mathbf{x}_0 \cdot \mathbf{e}_k \geq 0$ .
2. If  $\lambda^k \neq 0$ , then by complementary slackness we know  $\mathbf{x} \cdot \mathbf{e}_k = 0$ .

Combining these shows  $\mathbf{x} = \max(\mathbf{x}_0, \mathbf{0})$ , where the max is taken entrywise. In other words, the closest projection of  $\mathbf{x}_0$  onto the nonnegative vectors simply zeroes out negative entries.

#### 2.2.4 Integration

Our final task is to define a basic notion of an integral from multivariable calculus. Given a continuous function  $f : \mathbb{R}^n \rightarrow \mathbb{R}$ , we might ask for the integral  $\int_S f(\mathbf{x}) d\mathbf{x}$  over some subset  $S \subseteq \mathbb{R}^n$ . We will not get into the particularities of specifically which sets  $S$  are reasonable as domains of integration but rather assume here that  $S$  is not a pathological set over which integrals are not defined.

To begin, we might consider what it means to integrate  $f$  over a rectangle  $R = [a_1, b_1] \times [a_2, b_2] \times \dots \times [a_n, b_n]$ . In this case, we can define integration recursively using the *iterated integral*

$$\int_R f(\mathbf{x}) d\mathbf{x} := \int_{a_1}^{b_1} \int_{a_2}^{b_2} \dots \int_{a_n}^{b_n} f(x^1, \dots, x^n) dx^n \dots dx^1.$$

This is actually a recursive set of one-dimensional integrals rather than the integral of a function over a set in  $\mathbb{R}^n$ .

Given a more general set  $S \subseteq \mathbb{R}^n$ , define the *indicator function*

$$\chi_S(\mathbf{x}) := \begin{cases} 1 & \text{if } \mathbf{x} \in S \\ 0 & \text{otherwise.} \end{cases}$$

Then, we can define the integral of  $f$  over  $S$  as the integral of the product:

$$\int_S f(\mathbf{x}) d\mathbf{x} := \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \dots \int_{-\infty}^{\infty} f(x^1, \dots, x^n) \chi_S(x^1, \dots, x^n) dx^n \dots dx^1. \quad (2.14)$$

Once again, this iterated integral only requires nested calculations in one-dimension at a time. We will defer integration over more general domains like curves and surfaces until we need it.

## 2.3 EXERCISES

- 2.1. Show that an orthonormal basis of eigenvectors of an  $n \times n$  symmetric matrix  $A \succeq 0$  that spans  $\mathbb{R}^n$ .
- 2.2. Prove the following generalization of the spectral theorem: Suppose  $A, B \in \mathbb{R}^{n \times n}$  are symmetric and positive definite. Then, there exists a basis of generalized eigenvectors  $\{\mathbf{x}_1, \dots, \mathbf{x}_n\} \subset \mathbb{R}^n$  satisfying  $A\mathbf{x}_k = \lambda_k B\mathbf{x}_k$  for some  $\lambda_k \in \mathbb{R}$  that are orthogonal under the  $B$  inner product  $g_B(\mathbf{v}, \mathbf{w}) := \mathbf{v}^\top B\mathbf{w}$ .
- 2.3. **JS: Verify some matrix calculus identities.**
- 2.4. Suppose  $\mathbb{R}^n$  is equipped with a general inner product  $g(\cdot, \cdot)$ . Show that any linear operator  $L : \mathbb{R}^n \rightarrow \mathbb{R}^1$  can be written  $L(\mathbf{v}) = g(\mathbf{v}_0, \mathbf{v})$  for some fixed  $\mathbf{v}_0 \in \mathbb{R}^n$  depending on  $L$  and  $g$  but not  $\mathbf{v}$ . Use this fact to define a “generalized gradient vector” of  $f : \mathbb{R}^n \rightarrow \mathbb{R}$  with respect to inner product  $g$ , notated  $\nabla_g f(\mathbf{x})$ .
- 2.5. **JS: Minimax version of Lagrange/KKT**