Chapter 3

Matrices and Linear transformations

A linear transformation acting on a Euclidian vector can be represented as a matrix. Many of the concepts we introduce in this chapter generalize to linear operators acting on functions in infinite dimensional spaces, which is fundamental for the study of partial differential equations.

3.1 Matrix algebra

Linear transformation as a matrix

A function $f : \mathbb{R}^n \to \mathbb{R}^n$ is a *linear transformation*, or *linear map*, if

(i) $f(x + z) = f(x) + f(z)$,

(ii) $f(\alpha x) = \alpha f(x)$,

for all $x, z \in \mathbb{R}^n$ and $\alpha \in \mathbb{R}$. In the standard basis $(e_1, ..., e_n)$ we can express the ith component of the vector $y = f(x) \in \mathbb{R}^n$ as

$$y_i = f_i(x) = f_i(\sum_{j=1}^{n} x_j e_j) = \sum_{j=1}^{n} x_j f_i(e_j),$$

where $f_i : \mathbb{R}^n \to \mathbb{R}$ for all $i = 1, ..., n$. In component form, we write this as

$$\begin{aligned} y_1 &= a_{11}x_1 + ... + a_{1n}x_n \\ &\vdots \\ y_n &= a_{n1}x_1 + ... + a_{nn}x_n \end{aligned} \tag{3.1}$$

with $a_{ij} = f_i(e_j)$. That is $y = Ax$, where A is an $n \times n$ matrix

$$A = \begin{bmatrix} a_{11} & \cdots & a_{1n} \\ \vdots & \ddots & \vdots \\ a_{n1} & \cdots & a_{nn} \end{bmatrix}. \tag{3.2}$$

The set of real valued $m \times n$-matrices defines a vector space $\mathbb{R}^{m\times n}$, by the basic operations of (i) component-wise matrix addition and (ii) component-wise scalar multiplication. A matrix $A \in \mathbb{R}^{m\times n}$ also defines a *linear map* $x \mapsto Ax$, by the basic operations of the *matrix-vector product* and *component-wise scalar multiplication.*

$$\begin{aligned} A(x+y) &= Ax + Ay, \qquad && x, y \in \mathbb{R}^n, \\ A(\alpha x) &= \alpha Ax, && x \in \mathbb{R}^n, \alpha \in \mathbb{R}. \end{aligned}$$

Matrix-vector product

In *index notation* we write a vector $b = (b_i)$, and a matrix $A = (a_{ij})$, with i the *row index* and j is the *column index.* For an $m \times n$ matrix A, and x an n-dimensional column vector, we define the *matrix-vector product* $b = Ax$ to be the m-dimensional column vector

$$b_i = \sum_{j=1}^{n} a_{ij} x_j, \quad i = 1, ..., m. \tag{3.3}$$

With a_j the jth column of A, an m-vector, we can express the matrix-vector product as a linear combination of the set of column vectors $\{a_j\}_{j=1}^n$

$$b = Ax = \sum_{j=1}^{n} x_j a_j, \tag{3.4}$$

or in matrix form

$$\begin{bmatrix} \\ b \\ \\ \end{bmatrix} = \left[\begin{array}{c|c|c|c} & & & \\ a_1 & a_2 & \cdots & a_n \\ & & & \end{array}\right] \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = x_1 \begin{bmatrix} \\ a_1 \\ \\ \end{bmatrix} + x_2 \begin{bmatrix} \\ a_2 \\ \\ \end{bmatrix} + ... + x_n \begin{bmatrix} \\ a_n \\ \\ \end{bmatrix}.$$

The vector space spanned by $\{a_j\}_{j=1}^n$ is the *column space*, or *range*, of the matrix A, so that $\text{range}(A) = \text{span}\{a_j\}_{j=1}^n$. The *null space*, or *kernel*, of an $m \times n$ matrix A is the set of vectors $x \in \mathbb{R}^n$ such that $Ax = 0$, with 0 the zero vector in $\mathbb{R}^m$, that is $\text{null}(A) = \{x \in \mathbb{R}^n : Ax = 0\}$.

The dimension of the column space is the column *rank* of the matrix, $\text{rank}(A)$. We note that the column rank is equal to the row rank, corresponding to the space spanned by the row vectors of A, and the maximal rank of an $m \times n$ matrix is $\min(m, n)$, which we refer to as *full rank*.

Matrix-matrix product

The *matrix-matrix product* $B = AC$ is a matrix in $\mathbb{R}^{l \times n}$, defined for two matrices $A \in \mathbb{R}^{l \times m}$ and $C \in \mathbb{R}^{m \times n}$, as

$$b_{ij} = \sum_{k=1}^{m} a_{ik} c_{kj}, \tag{3.5}$$

with $B = (b_{ij})$, $A = (a_{ik})$ and $C = (c_{kj})$. Here we may sometimes omit the summation sign and use the *Einstein convention* where repeated indices imply summation over those same indices, so that we can express the matrix-matrix product (3.5) as $b_{ij} = a_{ik} c_{kj}$.

Similarly as for the matrix-vector product, we may interpret the columns b_j of the matrix-matrix product B as a linear combination of the columns a_k with coefficients c_{kj}

$$b_j = Ac_j = \sum_{k=1}^{m} c_{kj} a_k, \tag{3.6}$$

or in matrix form

$$\left[\begin{array}{c|c|c|c} & & & \\ b_1 & b_2 & \cdots & b_n \\ & & & \end{array}\right] = \left[\begin{array}{c|c|c|c} & & & \\ a_1 & a_2 & \cdots & a_m \\ & & & \end{array}\right] \left[\begin{array}{c|c|c|c} c_1 & c_2 & \cdots & c_n \end{array}\right].$$

For two linear transformations $f(x)$ and $g(x)$ on $\mathbb{R}^n$, with associated square $n \times n$-matrices A and C, the matrix-matrix product AC corresponds to the composition $f \circ g(x) = f(g(x))$.

Matrix transpose and the inner and outer products

The *transpose* (or *adjoint*) of an $m \times n$ matrix $A = (a_{ij})$ is defined as the matrix $A^T = (a_{ji})$, with the column and row indices reversed.

Using the matrix transpose, the inner product of two vectors $v, w \in \mathbb{R}^n$ can be expressed in terms of a matrix-matrix product $v^T w$, as

$$(v, w) = v^T w = \begin{bmatrix} v_1 & \cdots & v_n \end{bmatrix} \begin{bmatrix} w_1 \\ \vdots \\ w_m \end{bmatrix} = v_1 w_1 + ... + v_n w_n. \qquad (3.7)$$

Similarly, the *outer product*, or *tensor product*, of two vectors $v, w \in \mathbb{R}^n$, denoted by $v \otimes w$, is defined as the $m \times n$ matrix corresponding to the matrix-matrix product vw^T, that is

$$v \otimes w = vw^T = \begin{bmatrix} v_1 \\ \vdots \\ v_m \end{bmatrix} \begin{bmatrix} w_1 & \cdots & w_n \end{bmatrix} = \begin{bmatrix} v_1 w_1 & \cdots & v_1 w_n \\ \vdots & & \vdots \\ v_m v_1 & & v_m w_n \end{bmatrix}.$$

In tensor notation we can express the inner and the outer products as $(v, w) = v_i w_i$ and $v \otimes w = v_i w_j$.

The transpose has the property that $(AB)^T = B^T A^T$, and thus satisfies the equation $(Ax, y) = (x, A^T y)$, for any $x \in \mathbb{R}^n, y \in \mathbb{R}^m$, which follows from the definition of the inner product in Euclidian vector spaces, since

$$(Ax, y) = (Ax)^T y = x^T A^T y = (x, A^T y). \qquad (3.8)$$

A is said to be *symmetric* (or *self-adjoint*) if $A = A^T$, so that $(Ax, y) = (x, Ay)$. If in addition $(Ax, x) > 0$ for all non-zero $x \in \mathbb{R}^m$, we say that A is a *symmetric positive definite* matrix. A matrix is said to be *normal* if $A^T A = AA^T$.

Matrix norms

To measure the size of a matrix, we first introduce the *Frobenius norm*, corresponding to the l_2-norm of the matrix A interpreted as an mn-vector, that is

$$\|A\|_F = \left(\sum_{i=1}^{m} \sum_{j=1}^{n} |a_{ij}|^2 \right)^{1/2}. \qquad (3.9)$$

The Frobenius norm is the norm associated to the following inner product over the space $\mathbb{R}^{m \times n}$,

$$(A, B) = \mathrm{tr}(A^T B), \qquad (3.10)$$

with the *trace* of a square $n \times n$ matrix $C = (c_{ij})$ defined by

$$\mathrm{tr}(C) = \sum_{i=1}^{n} c_{ii}. \tag{3.11}$$

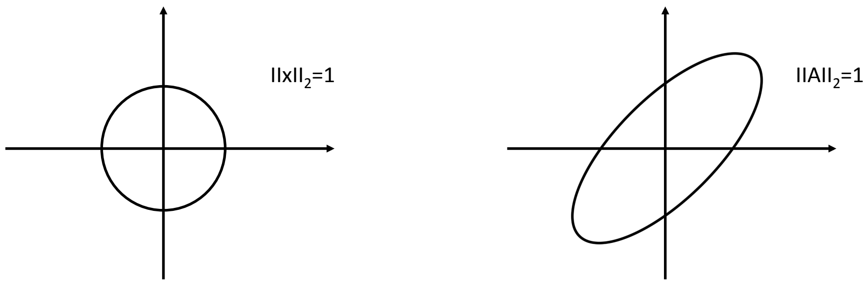

Figure 3.1: Illustration of the map $x \mapsto Ax$ through the unit circles $\|x\|_2 = 1$ (left) and $\|A\|_2 = 1$ (right), for the matrix A in (3.13).

Matrix norms for $A \in \mathbb{R}^{m \times n}$ are also induced by the respective l_p-norms on $\mathbb{R}^m$ and $\mathbb{R}^n$, in the form

$$\|A\|_p = \sup_{\substack{x \in \mathbb{R}^n \\ x \neq 0}} \frac{\|Ax\|_p}{\|x\|_p} = \sup_{\substack{x \in \mathbb{R}^n \\ \|x\|_p = 1}} \|Ax\|_p. \tag{3.12}$$

The last equality follows from the definition of a norm, and shows that the induced matrix norm can be defined in terms of its map of unit vectors, which we illustrate in Figure 3.1 and Figure 3.2 for the matrix

$$A = \begin{bmatrix} 1 & 2 \\ 0 & 2 \end{bmatrix}. \tag{3.13}$$

Determinant

The *determinant* of a square matrix A is denoted $\det(A)$ or $|A|$. For a 2×2 matrix we have the explicit formula

$$\det(A) = \begin{vmatrix} a & b \\ c & d \end{vmatrix} = ad - bc. \tag{3.14}$$

For example, for the matrix in (3.13) we have that $\det(A) = 1 \cdot 2 - 2 \cdot 0 = 2$.

The formula for the determinant is extended to a 3×3 matrix by

$$\det(A) = \begin{vmatrix} a & b & c \\ d & e & f \\ g & h & i \end{vmatrix} = a\begin{vmatrix} e & f \\ h & i \end{vmatrix} - b\begin{vmatrix} d & f \\ g & i \end{vmatrix} + c\begin{vmatrix} d & e \\ g & h \end{vmatrix}$$
$$= a(ei - fh) - b(di - fg) + c(dh - eg), \quad (3.15)$$

and by recursion this formula can be generalized to any square matrix.

For a 2×2 matrix the absolute value of the determinant equals to the area of the parallelogram that represents the image of the unit square under the map $x \mapsto Ax$, and similarly for a 3×3 matrix the volume of the mapped parallelepiped from the unit cube. More generally, the absolute value of the determinant represents a scale factor of the linear transformation A.

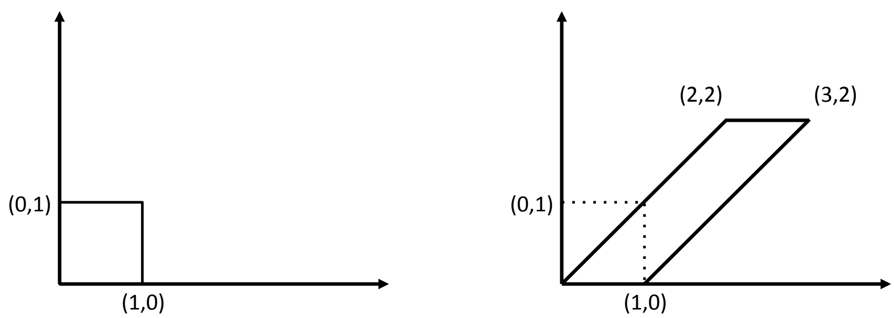

Figure 3.2: The map $x \mapsto Ax$ (right) of the unit square (left), for the matrix A in (3.13), with the corresponding area given by $|\det(A)| = 2$.

Matrix inverse

If the column vectors $\{a_j\}_{j=1}^n$ of a square $n \times n$ matrix form a basis for $\mathbb{R}^n$, then all vectors $b \in \mathbb{R}^n$ can be expressed as $b = Ax$, where $x \in \mathbb{R}^n$ is the vector of coordinates of b in the basis $\{a_j\}_{j=1}^n$. In particular, all $x \in \mathbb{R}^n$ can be expressed as $x = Ix$, where I is the square $n \times n$ *identity matrix* in $\mathbb{R}^n$, taking the standard basis as column vectors,

$$I = \begin{bmatrix} e_1 & e_2 & \cdots & e_n \end{bmatrix} = \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 0 & 1 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & 0 & 1 \end{bmatrix}.$$

A square matrix $A \in \mathbb{R}^{n\times n}$ is *invertible*, or *non-singular*, if there exists an *inverse matrix* $A^{-1} \in \mathbb{R}^{n\times n}$ such that $A^{-1}A = AA^{-1} = I$, which also means that $(A^{-1})^{-1} = A$. Further, for two matrices A and B we have the property that $(AB)^{-1} = B^{-1}A^{-1}$.

Theorem 4. *For a square matrix $A \in \mathbb{R}^{n\times n}$, the following is equivalent:*

(i) *A has an inverse A^{-1},*

(ii) $\det(A) \neq 0$,

(iii) $\text{rank}(A) = n$,

(iv) $\text{range}(A) = \mathbb{R}^n$

(v) $\text{null}(A) = \{0\}$.

The matrix inverse is unique. To see this, assume that there exist two matrices B_1 and B_2 such that $AB_1 = AB_2 = I$; which by linearity gives that $A(B_1 - B_2) = 0$, but since $\text{null}(A) = \{0\}$ we have that $B_1 = B_2$.

3.2 Some linear transformations

Affine transformations

An *affine transformation*, or *affine map*, is a linear transformation composed with a translation, corresponding to a matrix multiplication followed by vector addition. For example, counter-clockwise rotation of a vector by an angle θ in $\mathbb{R}^2$, takes the form of multiplication by a *Givens rotation* matrix,

$$A = \begin{bmatrix} \cos(\theta) & -\sin(\theta) \\ \sin(\theta) & \cos(\theta) \end{bmatrix}, \tag{3.16}$$

whereas translation corresponds to addition by a position vector b, so that the affine map takes the form $x \mapsto Ax + b$.

We note that any triangle is related to each other through an affine map; for example in the Euclidian plane $\mathbb{R}^2$, or to a surface (manifold) in Euclidian space $\mathbb{R}^3$, see Figure 3.3.

Remark 1. *We note that by using* homogeneous coordinates*, or* projective coordinates*, we can express any affine transformation as a matrix multiplication, including translation. In $\mathbb{R}^2$ a vector $x = (x_1, x_2)^T$ in standard*

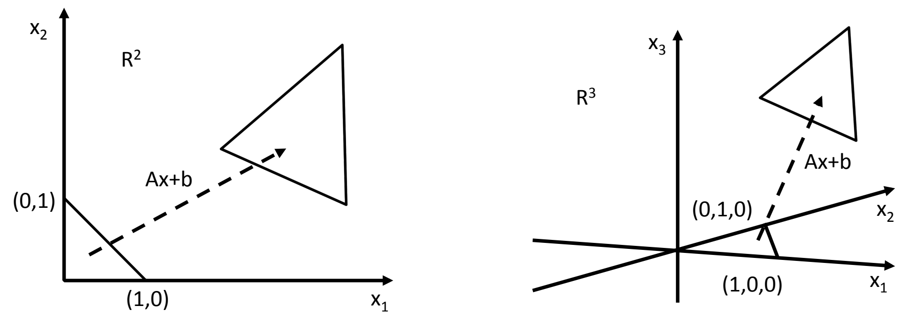

Figure 3.3: Affine maps $x \mapsto Ax + b$ of the *reference triangle* with corners in $(0,0)$, $(1,0)$, $(0,1)$; in $\mathbb{R}^2$ (left); to a surface (manifold) in $\mathbb{R}^3$ (right).

Cartesian coordinates, is represented as $x = (x_1, x_2, 1)^T$ *in homogeneous coordinates, so that the rotation matrix takes the form*

$$A = \begin{bmatrix} \cos(\theta) & -\sin(\theta) & 0 \\ \sin(\theta) & \cos(\theta) & 0 \\ 0 & 0 & 1 \end{bmatrix}, \tag{3.17}$$

and translation by a vector (t_1, t_2) *is expressed by the matrix*

$$A = \begin{bmatrix} 1 & 0 & t_1 \\ 0 & 1 & t_2 \\ 0 & 0 & 1 \end{bmatrix}. \tag{3.18}$$

Difference and summation matrices

Subdivide the interval $[0,1]$ into a *structured grid* with m intervals and $m+1$ *nodes* x_i, such that $0 = x_0 < x_1 < x_2 < ... < x_m = 1$, with a constant interval length $h = x_i - x_{i-1}$, so that $x_i = x_0 + ih$.

For each $x = x_i$ we may approximate the integral of a function $f(x)$ with $f(0) = 0$, by a rectangular quadrature rule, so that

$$F(x_i) = \int_0^{x_i} f(s)ds \approx \sum_{k=1}^{i} f(x_k)h = F_h(x_i), \tag{3.19}$$

which defines a function $F_h(x_i)$ for all nodes x_i in the subdivision. This linear transformation of the vector of sampled function values at the nodes

$y = (f(x_1), ..., f(x_m))^T$ can be expressed in the following matrix equation,

$$L_h y = \begin{bmatrix} h & 0 & \cdots & 0 \\ h & h & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ h & h & \cdots & h \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_m) \end{bmatrix} = \begin{bmatrix} f(x_1)h \\ f(x_1)h + f(x_2)h \\ \vdots \\ \sum_{k=1}^m f(x_k)h \end{bmatrix}, \tag{3.20}$$

where L_h is a summation matrix, with its inverse given by

$$L_h = h \begin{bmatrix} 1 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{bmatrix}, \quad L_h^{-1} = h^{-1} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ -1 & 1 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & -1 & 1 \end{bmatrix}. \tag{3.21}$$

The inverse matrix L_h^{-1} corresponds to a difference matrix over the same subdivision. To see this, multiply the matrix L_h^{-1} to $y = f(x_i)$,

$$L_h^{-1} y = h^{-1} \begin{bmatrix} 1 & 0 & \cdots & 0 \\ -1 & 1 & \cdots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & \cdots & -1 & 1 \end{bmatrix} \begin{bmatrix} f(x_1) \\ f(x_2) \\ \vdots \\ f(x_m) \end{bmatrix} = \begin{bmatrix} f(x_1)/h \\ (f(x_2) - f(x_1))/h \\ \vdots \\ (f(x_m) - f(x_{m-1}))/h \end{bmatrix}. \tag{3.22}$$

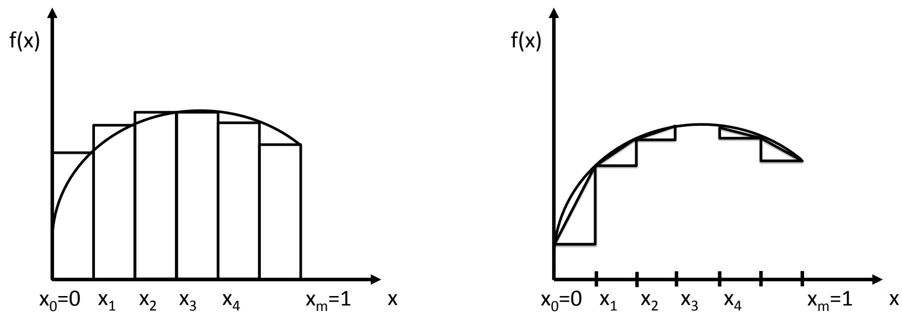

Figure 3.4: Rectangular rule quadrature (left) and finite difference approximation (right) on a subdivision of $[0, 1]$ with interval length h.

As the interval length $h \to 0$, the summation and difference matrices converge to integral and differential operators, such that for each $x \in (0, 1)$,

$$L_h y \to \int_0^x f(s)ds, \quad L_h^{-1} y \to f'(x). \tag{3.23}$$

Further, we have for the product of the two matrices that

$$y = L_h L_h^{-1} y \to f(x) = \int_a^x f'(s)ds, \tag{3.24}$$

as $h \to 0$, which corresponds to the *Fundamental theorem of Calculus.*

Difference operators

The matrix L_h^{-1} in (3.21) corresponds to a backward difference operator D_h^-, and similarly we can define a forward difference operator D_h^+, by

$$D_h^- = h^{-1}\begin{bmatrix} 1 & 0 & 0 & \cdots & 0 \\ -1 & 1 & 0 & \cdots & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & -1 & 1 & 0 \\ 0 & \cdots & 0 & -1 & 1 \end{bmatrix}, \quad D_h^+ = h^{-1}\begin{bmatrix} -1 & 1 & 0 & \cdots & 0 \\ 0 & -1 & 1 & \cdots & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & 0 & -1 & 1 \\ 0 & \cdots & 0 & 0 & -1 \end{bmatrix}.$$

The matrix-matrix product $D_h^+ D_h^-$ takes the form,

$$D_h^+ D_h^- = h^{-2}\begin{bmatrix} -1 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ \vdots & & & \ddots & \vdots \\ 0 & \cdots & 1 & -2 & 1 \\ 0 & \cdots & 0 & 1 & -2 \end{bmatrix}, \tag{3.25}$$

which corresponds to an approximation of a second order differential operator. The matrix $A = -D_h^+ D_h^-$ is *diagonally dominant*, that is

$$|a_{ii}| \geq \sum_{j \neq i} |a_{ij}|, \tag{3.26}$$

and symmetric positive definite, since

$$\begin{aligned} x^T A x &= ... + x_i(-x_{i-1} + 2x_i - x_{i+1}) + ... + x_n(-x_{n-1} + 2x_n) \\ &= ... - x_i x_{i-1} + 2x_i^2 - x_i x_{i+1} - x_{i+1} x_i + ... - x_{n-1} x_n + 2x_n^2 \\ &= ... + (x_i - x_{i-1})^2 + (x_{i+1} - x_i)^2 + ... + x_n^2 > 0, \end{aligned}$$

for any non-zero vector x.

Since the second order difference matrix $A = -(D_h^+ D_h^-)$ is symmetric positive definite, there exists a unique invers A^{-1}. For example, in the case of a 5×5 matrix we have that

$$A = 1/h^2 \begin{bmatrix} 2 & -1 & 0 & 0 & 0 \\ -1 & 2 & -1 & 0 & 0 \\ 0 & -1 & 2 & -1 & 0 \\ 0 & 0 & -1 & 2 & -1 \\ 0 & 0 & 0 & -1 & 2 \end{bmatrix}, \quad A^{-1} = h^2/6 \begin{bmatrix} 5 & 4 & 3 & 2 & 1 \\ 4 & 8 & 6 & 4 & 2 \\ 3 & 6 & 9 & 6 & 3 \\ 2 & 4 & 6 & 8 & 4 \\ 1 & 2 & 3 & 4 & 5 \end{bmatrix},$$

where we note that while the second order difference operator A is a *sparse matrix* with only few non-zero elements, the inverse A^{-1} is a *full matrix* without zero elements, corresponding to a weighted integral (summation) operator.

The finite difference method

For a vector $y = u(x_i)$, the ith row of the matrix $D_h^+ D_h^-$ corresponds to a *finite difference stencil*, with $u(x_i)$ function values sampled at the nodes x_i of the structured grid representing the subdivision of the interval $I = (0, 1)$,

$$\begin{aligned} [(D_h^+ D_h^-)y]_i &= \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2} \\ &= \frac{\dfrac{u(x_{i+1}) - u(x_i)}{h} - \dfrac{u(x_i) - u(x_{i-1})}{h}}{h}. \end{aligned}$$

Similarly, the difference operators D_h^- and D_h^+ correspond to finite difference stencils over the grid, and we have that for $x \in I$,

$$(D_h^+ D_h^-)y \to u''(x), \quad (D_h^-)y \to u'(x), \quad (D_h^+)y \to u'(x), \tag{3.27}$$

as the grid size $h \to 0$.

The *finite difference method* for solving differential equations is based on approximation of differential operators by such difference stencils over a grid. We can thus, for example, approximate the differential equation

$$-u''(x) + u(x) = f(x), \tag{3.28}$$

by the matrix equation

$$-(D_h^+ D_h^-)y + (D_h^-)y = b, \tag{3.29}$$

with $b_i = f(x_i)$. The finite difference method extends to multiple dimensions, where the difference stencils are defined over structured Cartesian grids in $\mathbb{R}^2$ or $\mathbb{R}^3$.

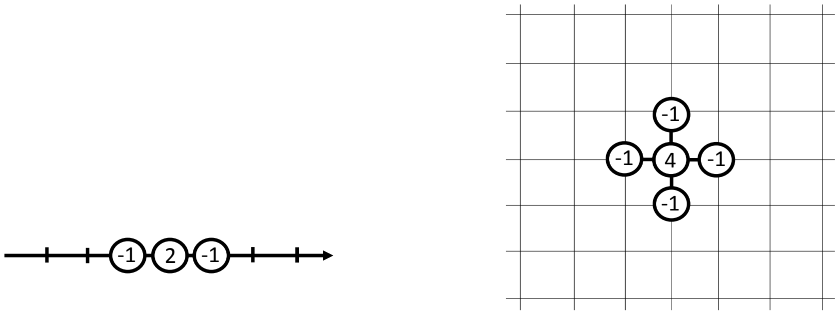

Figure 3.5: Example of finite difference stencils corresponding to the difference operator $-(D_h^+ D_h^-)$ over structured grids in $\mathbb{R}$ (left) and $\mathbb{R}^2$ (right).

Convolution

3.3 Orthogonal projectors

Orthogonal matrix

A square matrix $Q \in \mathbb{R}^{n\times n}$ is *ortogonal*, or *unitary*, if $Q^T = Q^{-1}$. With q_j the columns of Q we thus have that $Q^T Q = I$, or in matrix form,

$$\begin{bmatrix} \quad q_1 \quad \\ \hline q_2 \\ \hline \vdots \\ \hline q_n \end{bmatrix} \left[\begin{array}{c|c|c|c} q_1 & q_2 & \cdots & q_n \end{array} \right] = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & & \ddots & \\ & & & 1 \end{bmatrix},$$

so that the columns q_j form an orthonormal basis for $\mathbb{R}^n$.

Multiplication by an orthogonal matrix preserves the angle between two vectors $x, y \in \mathbb{R}^n$, since

$$(Qx, Qy) = (Qx)^T Qy = x^T Q^T Qy = x^T y = (x, y), \tag{3.30}$$

and thus also the length of a vector,

$$\|Qx\| = (Qx, Qx)^{1/2} = (x, x)^{1/2} = \|x\|. \tag{3.31}$$

As a linear transformation an orthogonal matrix acts as a rotation or reflection, depending on the sign of the determinant which is always either 1 or -1.

Orthogonal projector

A *projection matrix*, or *projector*, is a square matrix P such that

$$P^2 = PP = P. \tag{3.32}$$

It follows that

$$Pv = v, \tag{3.33}$$

for all vectors $v \in \text{range}(P)$, since v is of the form $v = Px$ for some x, and thus $Pv = P^2x = Px = v$. For $v \notin \text{range}(P)$ we have that $P(Pv - v) = P^2v - Pv = 0$, so that the projection error $Pv - v \in \text{null}(P)$.

The matrix $I - P$ is also a projector, the *complementary projector* to P, since $(I - P)^2 = I - 2P + P^2 = I - P$. The range and null space of the two projectors are related as $\text{range}(I - P) = \text{null}(P)$ and $\text{range}(P) = \text{null}(I - P)$, so that P and $I - P$ separates $\mathbb{R}^n$ into two subspaces S_1 and S_2, since the only $v \in \text{range}(P) \cap \text{range}(I - P)$ is the zero vector; $v = v - Pv = (I - P)v = \{0\}$.

If the two subspaces S_1 and S_2 are orthogonal, we say that P is an *orthogonal projector*. This is equivalent to the condition $P = P^T$, since the inner product between two vectors in S_1 and S_2 then vanish,

$$(Px, (I - P)y) = (Px)^T(I - P)y = x^TP^T(I - P)y = x^T(P - P^2)y = 0.$$

If P is an orthogonal projector, so is $I - P$. For example, the orthogonal projection P_yx of one vector x in the direction of another vector y, its orthogonal complement $P^{\perp y}x$, and P_y^rx, its reflection in y, correspond to the projectors

$$P_y = \frac{yy^T}{\|y\|^2}, \quad P^{\perp y} = I - \frac{yy^T}{\|y\|^2}, \quad P_y^r = I - 2\frac{yy^T}{\|y\|^2}. \tag{3.34}$$

Gram-Schmidt orthogonalization

For a square matrix $A \in \mathbb{R}^{n\times n}$ we denote the successive vector spaces spanned by its column vectors a_j as

$$\langle a_1\rangle \subseteq \langle a_1, a_2\rangle \subseteq \langle a_1, a_2, a_3\rangle \subseteq ... \subseteq \langle a_1, ..., a_m\rangle. \tag{3.35}$$

Assuming that A has full rank, we now ask if we for each such vector space can construct an orthonormal basis q_j such that $\langle q_1, ..., q_j\rangle = \langle a_1, ..., a_j\rangle$, for all $j \leq n$.

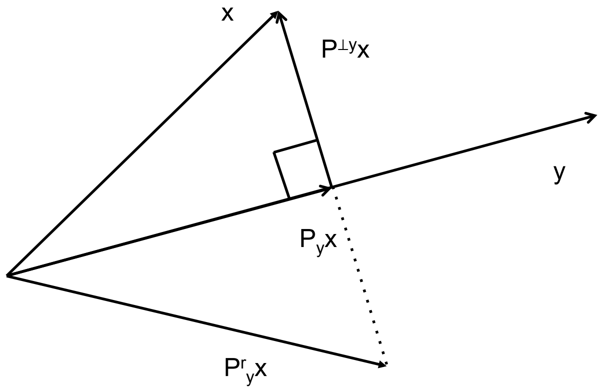

Figure 3.6: The projector $P_y x$ of one vector x in the direction of another vector y, its orthogonal complement $P^{\perp y}x$, and the reflector $P^r_y x$.

Given a_j, we can successively construct vectors v_j that are orthogonal to the spaces $\langle q_1, ..., q_{j-1}\rangle$, since by (2.13) we have that

$$v_j = a_j - \sum_{i=1}^{j-1} (a_j, q_i) q_i, \tag{3.36}$$

for all $j = 1, ..., n$, where each vector is then normalized to get $q_j = v_j/\|v_j\|$. This is the *classical Gram-Schmidt iteration*.

With $\hat{Q}_{j-1}$ the $n \times j-1$ matrix consiting of the orthogonal column vectors q_i, we can rewrite (3.36) in terms of an orthogonal projector P_j,

$$v_j = a_j - \sum_{i=1}^{j-1} (a_j, q_i) q_i = a_j - \sum_{i=1}^{j-1} q_i q_i^T a_j = (I - \hat{Q}_{j-1}\hat{Q}_{j-1}^T) a_j = P_j a_j,$$

with $\hat{Q}_{j-1}\hat{Q}_{j-1}^T$ an orthogonal projector onto range($\hat{Q}_{j-1}$), the column space of $\hat{Q}_{j-1}$, and $P_j = I - \hat{Q}_{j-1}\hat{Q}_{j-1}^T$ an orthogonal projector onto the space orthogonal to range($\hat{Q}_{j-1}$), with $P_1 = I$. Thus the Gram-Schmidt iteration can be expressed in terms of the projector P_j as $q_j = P_j a_j/\|P_j a_j\|$, for $j = 1, ..., n$.

Alternatively, P_j can be constructed by successive multiplication of projectors $P^{\perp q_i} = I - q_i q_i^T$, orthogonal to each individual vector q_i, such that

$$P_j = P^{\perp q_{j-1}} \cdots P^{\perp q_2} P^{\perp q_1}. \tag{3.37}$$

The *modified Gram-Schmidt iteration* corresponds to instead using this formula to construct P_j, which leads to a more robust algorithm that the classical Gram-Schmidt iteration.

Algorithm 1: Modified Gram-Schmidt iteration

```
for i = 1 to n do
    v_i = a_i
end
for i = 1 to n do
    r_ii = ||v_i||
    q_i = v_i / r_ii
    for j = 1 to i + 1 do
        r_ij = q_i^T v_j
        v_j = v_j - r_ij q_i
    end
end
```

3.4 QR factorization

By introducing the notation $r_{ij} = (a_j, q_i)$ and $r_{ii} = \|a_j - \sum_{i=1}^{j-1}(a_j, q_i)q_i\|$, we can rewrite the Gram-Schmidt iteration (3.36) as

$$\begin{aligned} a_1 &= r_{11}q_1 \\ a_2 &= r_{12}q_1 + r_{22}q_2 \\ &\vdots \\ a_n &= r_{1n}q_1 + ... + r_{2n}q_n \end{aligned} \tag{3.38}$$

which corresponds to the QR factorization $A = QR$, with Q an orthogonal matrix and R an upper triangular matrix, that is

$$\left[\begin{array}{c|c|c|c} a_1 & a_2 & \cdots & a_n \end{array}\right] = \left[\begin{array}{c|c|c|c} q_1 & q_2 & \cdots & q_n \end{array}\right] \begin{bmatrix} r_{11} & r_{12} & \cdots & r_{1n} \\ & r_{22} & & \\ & & \ddots & \vdots \\ & & & r_{nn} \end{bmatrix}.$$

Existence and uniqueness of the QR factorization of a non-singular matrix A follows by construction from Algorithm 1.

The modified Gram-Schmidt iteration of Algorithm 1 corresponds to successive multiplication of upper triangular matrices R_k on the right of the matrix A, such that the resulting matrix Q is an orthogonal matrix,

$$AR_1R_2\cdots R_n = Q, \tag{3.39}$$

and with the notation $R^{-1} = R_1R_2\cdots R_n$, the matrix $R = (R^{-1})^{-1}$ is also an upper triangular matrix.

3.5 Exercises

Problem 8. *Prove the equivalence of the definitions of the induced matrix norm, defined by*

$$\|A\|_p = \sup_{\substack{x\in\mathbb{R}^n \\ x\neq 0}} \frac{\|Ax\|_p}{\|x\|_p} = \sup_{\substack{x\in\mathbb{R}^n \\ \|x\|_p=1}} \|Ax\|_p. \tag{3.40}$$