Matrix and Calculus Refresher

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Welcome

The Matrix and Calculus Refresher notes were written by Korbinian Strimmer from 2018–2025. This version is from 5 November 2025.

If you have any questions, comments, or corrections please get in touch! [1]

Updates

The notes will be updated from time to time.

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Preface

About the author

Hello! My name is Korbinian Strimmer and I am a Professor in Statistics. I am a member of the Statistics group at the Department of Mathematics of the University of Manchester. You can find more information about me on my home page.

About the notes

In statistics and machine learning we make frequent use of matrix notation, algebra, decompositions and vector and matrix calculus. The aim of these supplementary notes is to provide a refresher for students to quickly gain a working knowledge about matrices and the calculus of functions with several variables.

The notes are supporting information for a number of lecture courses in statistics that I teach or have taught at the Department of Mathematics of the University of Manchester.

This includes the currently offered modules:

- MATH27720 Statistics 2: Likelihood and Bayes and
- MATH38161 Multivariate Statistics,

as well as the retired module (not offered any more):

- MATH20802 Statistical Methods.

1 Matrix essentials

1.1 Overview

In statistics we will frequently make use of matrix calculations and matrix notation.

Throughout we mostly work with **real matrices**, i.e. we assume all matrix elements are real numbers. However, one important matrix decomposition — the eigenvalue decomposition — can yield complex-valued matrices even when applied to real matrices. Thus occasionally we will also need to deal also with complex numbers.

For further details on matrix theory please consult the lecture notes of related modules (e.g. linear algebra).

1.2 Matrix basics

Matrix notation

In matrix notation we distinguish between scalars, vectors, and matrices:

Scalar: x, X, lower or upper case, plain type.

Vector: $\boldsymbol{x}$, lower case, bold type. In handwriting an arrow $\vec{x}$ indicates a vector.

By default, a vector is a column vector with its elements arranged in a column and the index of the components x_i refers to the row:

$$\boldsymbol{x} = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix}$$

In a row vector $x^T = (x_1, \ldots, x_m)$ the elements are arranged in a row and the index of the component x_j refers to the column.

The **transpose** operator (indicated by the superscript T) converts a column vector into a row vector, and vice versa. To save space we may conveniently write a column vector $x = (x_1, \ldots, x_n)^T$ as transposed row vector.

Matrix: X, upper case, bold type. In handwriting an underscore $\underline{X}$ indicates a matrix.

In component notation we write $X = (x_{ij})$. By convention, the first index (here i) of the scalar elements x_{ij} denotes the row and the second index (here j) the column of the matrix. For n rows and m columns we can view the matrix $X = (x_1, \ldots, x_m)$ either as being composed of m column vectors $x_j = \begin{pmatrix} x_{1j} \\ \vdots \\ x_{nj} \end{pmatrix}$, or the same matrix $X = \begin{pmatrix} z_1^T \\ \vdots \\ z_n^T \end{pmatrix}$ as being composed of n row vectors $z_i^T = (x_{i1}, \ldots, x_{im})$.

A (column) vector of dimension n is a matrix of size $n \times 1$. A row vector of dimension m is a matrix of size $1 \times m$. A scalar is of dimension 1 and is a matrix of size 1×1.

Notation for random vectors and matrices

A **random matrix** (vector) is a matrix (vector) whose elements are random variables.

It is common practise in univariate statistics to distinguish random variables and their fixed realisations by using upper case versus lower case. However, this convention breaks down when working with matrices and vectors.

Therefore, when working with multivariate random quantities it is best practise (see e.g. Mardia et al. 1979)[1] to always state explicitly whether a matrix, vector or scalar is a random variable, especially when this is not obvious from the context.

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[1] Mardia, K. V., J. T. Kent and J. M. Bibby. 1979. *Multivariate Analysis*. Academic Press.

Special matrices

The matrix or vector **1** consists entirely of ones as its elements. Most often it is used in the form of a column vector with n rows:

$$\mathbf{1}_n = \begin{pmatrix} 1 \\ 1 \\ 1 \\ \vdots \\ 1 \end{pmatrix}$$

Similarly, **0** is a matrix or vector that contains only zeros as its elements. Most often it is used in the form of a column vector with n rows:

$$\mathbf{0}_n = \begin{pmatrix} 0 \\ 0 \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

A **diagonal matrix** is a matrix where all off-diagonal elements are zero. By $\mathrm{Diag}(a_1, \ldots, a_n)$ or $\mathrm{Diag}(a)$ a diagonal matrix is specified by listing its diagonal elements. Applied to a matrix $\mathrm{Diag}(A)$ returns its diagonal elements as a vector.

I_n is the **identity matrix**. It is a square matrix of size $n \times n$ with the diagonal filled with 1 and off-diagonals filled with 0.

$$I_n = \mathrm{Diag}(\mathbf{1}_n) = \begin{pmatrix} 1 & 0 & 0 & \ldots & 0 \\ 0 & 1 & 0 & \ldots & 0 \\ 0 & 0 & 1 & & 0 \\ \vdots & \vdots & & \ddots & \\ 0 & 0 & 0 & & 1 \end{pmatrix}$$

Any matrix can be partitioned into blocks or sub-matrices. A **block-structured matrix** or **block matrix** partitioning rows and columns into two groups has the form

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where A_{11}, A_{22}, A_{12} and A_{21} are themselves matrices. If A is symmetric (hence square) then A_{11} and A_{22} must also be symmetric and $A_{21} = A_{12}^T$.

A **block diagonal** matrix is a symmetric block matrix with vanishing off-diagonal blocks and symmetric sub-matrices along the diagonal.

A **triangular matrix** is a square matrix whose elements either below or above the diagonal are all zero (upper vs. lower triangular matrix).

1.3 Simple matrix operations

Matrix addition and multiplication

Matrices behave much like common numbers. For example, we can add matrices $C = A + B$ and multiply matrices $C = AB$.

For **matrix addition** $C = A + B$ we add the corresponding elements $c_{ij} = a_{ij} + b_{ij}$. For matrix addition A and B must have the same dimensions, i.e. the same number of rows and columns.

The **dot product**, or **scalar product**, of two vectors a and b is a scalar given by $a \cdot b = \langle a, b \rangle = a^T b = b^T a = \sum_{i=1}^{d} a_i b_i$.

Matrix multiplication $C = AB$ is obtained by setting $c_{ij} = \sum_{k=1}^{m} a_{ik} b_{kj}$ where m is the number of columns of A and the number of rows in B. Thus, C contains all possible dot products of the row vectors in A with the column vectors in B. For matrix multiplication the number of columns in A must match the number of rows in B. Note that matrix multiplication in general (for $m > 1$) does not commute, i.e. $AB \neq BA$.

Matrix transpose

The matrix transpose A^T indicate by the superscript T interchanges rows and columns of a matrix. The transpose is a linear operator $(A + B)^T = A^T + B^T$ and applied to a matrix product it reverses the ordering, therefore $(AB)^T = B^T A^T$.

If $A = A^T$ then A is symmetric (and square).

For a rectangular matrix A the matrices $A^T A$ and $A A^T$ are square and symmetric with non-negative diagonal.

Matrix vectorisation

The vectorisation operator $\text{Vec}(A)$ converts the matrix A of dimension $n \times m$ into a vector of dimension nm by stacking the m column vectors of $A = (a_1, \ldots, a_m)$ on top of each other:

$$\text{Vec}(A) = \begin{pmatrix} a_1 \\ a_2 \\ \vdots \\ a_m \end{pmatrix}$$

1.4 Matrix summaries

Row, column and grand sum

Assume a matrix A of size $n \times m$.

The sum over the m entries of row i is $\sum_{j=1}^{m} a_{ij}$. In matrix notation the n row sums are given by $A\mathbf{1}_m$.

The sum over the n entries of column j is $\sum_{i=1}^{n} a_{ij}$. In matrix notation the m column sums are $A^T\mathbf{1}_n$.

The grand sum of all matrix entries of A is obtained by

$$\sum_{i=1}^{n}\sum_{j=1}^{m} a_{ij} = \mathbf{1}_n^T A \mathbf{1}_m$$

Matrix trace

The trace of the matrix is the sum of the diagonal elements $\text{Tr}(A) = \sum a_{ii}$.

The trace is invariant against transposition, i.e.

$$\text{Tr}(A) = \text{Tr}(A^T)$$

A useful identity for the matrix trace of the product of two matrices is

$$\text{Tr}(AB) = \text{Tr}(BA)$$

Intriguingly, the trace of a matrix equals the sum of the eigenvalues of the matrix (see further below).

Row, column and grand sum of squares

The sum over the m squared entries of row i is $\sum_{j=1}^{m} a_{ij}^2$. In matrix notation the n row sums of squares are given by $\mathrm{Diag}(AA^T)$.

The sum over the n squared entries of column j is $\sum_{i=1}^{n} a_{ij}^2$. In matrix notation the m column sums of squares are $\mathrm{Diag}(A^T A)$.

The grand sum of all squared elements of A is obtained by

$$\sum_{i=1}^{n} \sum_{j=1}^{m} a_{ij}^2 = \mathrm{Tr}(A^T A) = \mathrm{Tr}(AA^T)$$
$$= \mathrm{Vec}(A)^T \mathrm{Vec}(A)$$

This is also known as the squared Frobenius norm of A (see below).

Sum of squared diagonal entries

The sum of the squared entries on the diagonal is in matrix notation

$$\mathrm{Diag}(A)^T \mathrm{Diag}(A) = \sum_{i=1}^{\min(n,m)} a_{ii}^2$$

Frobenius inner product

The **Frobenius inner product** between two rectangular matrices A and B of the *same dimension* is the scalar

$$\langle A, B \rangle = \mathrm{Tr}(AB^T) = \mathrm{Tr}(BA^T)$$
$$= \mathrm{Tr}(A^T B) = \mathrm{Tr}(B^T A)$$
$$= \mathrm{Vec}(A)^T \mathrm{Vec}(B)$$
$$= \sum_{i,j} a_{ij} b_{ij} \, .$$

This generalises the dot product between two vectors. Note that the dot product can therefore also be written as the trace of a matrix

$$\langle a, b \rangle = \mathrm{Tr}(ab^T) = \mathrm{Tr}(ba^T) \, .$$

Euclidean norm

The **squared Euclidean norm** or the **squared length** of the vector a is the dot product $||a||_2^2 = a \cdot a = \langle a, a \rangle = a^T a = a a^T = \sum_{i=1}^d a_i^2$.

The **squared Frobenius norm** is a generalisation of the squared Euclidean vector norm to a rectangular matrix and is the sum of the squares of all its elements. Using the trace it can be written as

$$
\begin{aligned}
||A||_F^2 &= \langle A, A \rangle \\
&= \text{Tr}(A^T A) = \text{Tr}(AA^T) \\
&= \text{Vec}(A)^T \text{Vec}(A) \\
&= \sum_{i,j} a_{ij}^2 \, .
\end{aligned}
$$

A useful identity for the **squared Frobenius norm of the difference of two matrices** is

$$
\begin{aligned}
||A - B||_F^2 &= ||A||_F^2 + ||B||_F^2 - 2\langle A, B \rangle \\
&= \langle A, A \rangle + \langle B, B \rangle - 2\langle A, B \rangle \\
&= \text{Tr}(A^T A) + \text{Tr}(B^T B) - 2\,\text{Tr}(A^T B) \\
&= \sum_{i,j} (a_{ij} - b_{ij})^2 \, .
\end{aligned}
$$

The Frobenius norm of a matrix $||A||_F$ is not to be confused with the induced 2-norm of a matrix $||A||_2$. The latter equals the maximum absolute eigenvalue of the matrix, with $||A||_2 \leq ||A||_F$.

Determinant of a matrix

If A is a square matrix the determinant $\det(A)$ is a scalar measuring the volume spanned by the column vectors in A with the sign determined by the orientation of the vectors.

If $\det(A) \neq 0$ the matrix A is non-singular or non-degenerate. Conversely, if $\det(A) = 0$ the matrix A is singular or degenerate.

Intriguingly, the determinant of A is the product of the eigenvalues of A (see further below).

One way to compute the determinant of a matrix A is the Laplace cofactor expansion approach that proceeds recursively based on the determinants

of the sub-matrices $A_{-i,-j}$ obtained by deleting row i and column j from A. Specifically, at each level we compute the

1) cofactor expansion either

   a) along the i-th row — pick any row i:

$$\det(A) = \sum_{j=1}^{d} a_{ij}(-1)^{i+j}\det(A_{-i,-j}) \text{, or}$$

   b) along the j-th column — pick any j:

$$\det(A) = \sum_{i=1}^{d} a_{ij}(-1)^{i+j}\det(A_{-i,-j})$$

.

2) Then repeat until the sub-matrix is a scalar a and $\det(a) = a$.

The recursive nature of this algorithm leads to a complexity of order $O(d!)$ so it is not practical except for very small d. Therefore, in practice other more efficient algorithms for computing determinants are used but these still have algorithmic complexity in the order of $O(d^3)$ so for large dimensions obtaining determinants is very expensive.

However, some specially structured matrices do allow for very fast calculation.

The determinant of a **triangular matrix** (and thus also of a **diagonal matrix**)

$$A = \begin{pmatrix} a_{11} & 0 & \cdots & 0 \\ a_{21} & a_{22} & \cdots & 0 \\ \vdots & \vdots & \ddots & 0 \\ a_{d1} & a_{d2} & \cdots & a_{dd} \end{pmatrix}$$

is the product of its diagonal elements, i.e. $\det(A) = \prod_{i=1}^{d} a_{ii}$.

For a two-dimensional matrix $A = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}$ the determinant is $\det(A) = a_{11}a_{22} - a_{12}a_{21}$.

For a block-structured square matrix

$$A = \begin{pmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{pmatrix},$$

where the matrices on the diagonal A_{11} and A_{22} are themselves square but A_{12} and A_{21} may be rectangular, the determinant is

$$\det(A) = \det(A_{22})\det(C_1) = \det(A_{11})\det(C_2)$$

with the (Schur complement of A_{22})

$$C_1 = A_{11} - A_{12}A_{22}^{-1}A_{21}$$

and (Schur complement of A_{11})

$$C_2 = A_{22} - A_{21}A_{11}^{-1}A_{12}$$

Note that C_1 and C_2 are square matrices.

For a block-diagonal matrix A with $A_{12} = 0$ and $A_{21} = 0$ the determinant is $\det(A) = \det(A_{11})\det(A_{22})$, i.e. the product of the determinants of the sub-matrices along the diagonal.

Determinants have a multiplicative property,

$$\det(AB) = \det(BA) = \det(A)\det(B).$$

In the above A and B are both square and of the same dimension.

For rectangular A ($n \times m$) and rectangular B ($m \times n$) with $m \geq n$ this generalises to the Cauchy-Binet formula

$$\det(AB) = \sum_w \det(A_{,w})\det(B_{w,})$$

where the summation is over all $\binom{m}{n}$ index subsets w of size n taken from $\{1, \ldots, m\}$ keeping the ordering and $A_{,w}$ and $B_{w,}$ are the corresponding square $n \times n$ sub-matrices. If $m < n$ then $\det(AB) = 0$.

For scalar a $\det(aB) = a^d \det(B)$ where d is the dimension of B.

Another important identity is

$$\det(I_n + AB) = \det(I_m + BA)$$

where A and B are rectangular matrices. This is called the Weinstein-Aronszajn determinant identity (also credited to Sylvester).

1.5 Matrix inverse

Inversion of square matrix

If A is a square matrix then the inverse matrix A^{-1} is a matrix such that

$$A^{-1}A = AA^{-1} = I.$$

Only non-singular matrices with $\det(A) \neq 0$ are invertible.

As $\det(A^{-1}A) = \det(I) = 1$ the determinant of the inverse matrix equals the inverse determinant,

$$\det(A^{-1}) = \det(A)^{-1}.$$

The transpose of the inverse is the inverse of the transpose as

$$\begin{aligned}(A^{-1})^T &= (A^{-1})^T A^T (A^T)^{-1} \\ &= (AA^{-1})^T (A^T)^{-1} = (A^T)^{-1}.\end{aligned}$$

The inverse of a matrix product $(AB)^{-1} = B^{-1}A^{-1}$ is the product of the individual matrix inverses in reverse order.

There are many different algorithms to compute the inverse of a matrix (which is essentially a problem of solving a system of equations). The computational complexity of matrix inversion is of the order $O(d^3)$ where d is the dimension of A. Therefore matrix inversion is very costly in higher dimensions.

Example 1.1. Inversion of a 2×2 matrix:

The inverse of the matrix $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}$ is $A^{-1} = \frac{1}{ad-bc} \begin{pmatrix} d & -b \\ -c & a \end{pmatrix}$

Inversion of structured matrices

However, for specially structured matrices inversion can be done effectively:

- The inverse of a **diagonal matrix** is another diagonal matrix obtained by inverting the diagonal elements.
- More generally, the inverse of a **block-diagonal matrix** is obtained by individually inverting the blocks along the diagonal.

The **Woodbury matrix identity** simplifies the inversion of matrices that can be written as $A + UBV$ where A and B are both square and U and V are suitable rectangular matrices:

$$(A + UBV)^{-1} = A^{-1} - A^{-1}U(B^{-1} + VA^{-1}U)^{-1}VA^{-1}$$

Typically, the inverse A^{-1} is either already known or can be easily obtained and the dimension of B is much lower than that of A.

The class of matrices that can be most easily inverted are **orthogonal matrices** whose inverse is obtained simply by transposing the matrix.

1.6 Orthogonal matrices

Properties

An orthogonal matrix Q is a square matrix with the property that $Q^T = Q^{-1}$, i.e. the transpose is also the inverse. This implies that $QQ^T = Q^TQ = I$.

Both the column and the row vectors in Q all have length 1. This implies that each element q_{ij} of Q can only take a value in the interval $[-1, 1]$.

The identity matrix I is the simplest example of an orthogonal matrix.

The squared Euclidean and Frobenius norm is preserved when a vector a or matrix A is multiplied with an orthogonal matrix Q:

$$||Qa||_2^2 = (Qa)^T Qa = a^T a = ||a||_2^2$$

and

$$||QA||_F^2 = \text{Tr}\left((QA)^T QA\right) = \text{Tr}\left(A^T A\right) = ||A||_F^2$$

Multiplication of Q with a vector results in a new vector of the same length but with a change in direction (unless $Q = I$). An orthogonal matrix Q can thus be interpreted geometrically as an operator performing rotation, reflection and/or permutation.

The product $Q_3 = Q_1 Q_2$ of two orthogonal matrices Q_1 and Q_2 yields another orthogonal matrix as $Q_3 Q_3^T = Q_1 Q_2 (Q_1 Q_2)^T = Q_1 Q_2 Q_2^T Q_1^T = I$.

The determinant $\det(Q)$ of an orthogonal matrix is either +1 or -1, because $QQ^T = I$ and thus $\det(Q)\det(Q^T) = \det(Q)^2 = \det(I) = 1$.

The set of all orthogonal matrices of dimension d together with multiplication form a group called the orthogonal group $O(d)$. The subset of orthogonal matrices with $\det(Q) = 1$ are called rotation matrices and form with multiplication the special orthogonal group $SO(d)$. Orthogonal matrices with $\det(Q) = -1$ are rotation-reflection matrices.

Semi-orthogonal matrices

A rectangular $d \times k$ matrix Q is semi-orthogonal if for $k < d$ the k column vectors are orthonormal and hence $Q^T Q = I_k$, or if for $k > d$ the d row vectors are orthonormal with $QQ^T = I_d$.

The set of all (semi)-orthogonal matrices Q with $k \leq d$ column vectors is known as the Stiefel manifold St(d, k).

Generating orthogonal matrices

In two dimensions ($d = 2$) all orthogonal matrices R representing rotations with $\det(R) = 1$ are given by

$$R(\theta) = \begin{pmatrix} \cos \theta & -\sin \theta \\ \sin \theta & \cos \theta \end{pmatrix}$$

and those representing rotation-reflections G with $\det(G) = -1$ by

$$G(\theta) = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix} .$$

Every orthogonal matrix of dimension $d = 2$ can be represented as the product of at most two rotation-reflection matrices because

$$R(\theta) = G(\theta)\,G(0) = \begin{pmatrix} \cos \theta & \sin \theta \\ \sin \theta & -\cos \theta \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} .$$

Thus, the matrix G is a generator of two-dimensional orthogonal matrices. Note that $G(\theta)$ is symmetric, orthogonal and has determinant -1.

More generally, and applicable in arbitrary dimension, the role of generator is taken by the Householder reflection matrix

$$Q_{HH}(v) = I - 2vv^T$$

where v is a vector of unit length (with $v^T v = 1$) orthogonal to the reflection hyperplane. Note that $Q_{HH}(v) = Q_{HH}(-v)$. By construction the matrix $Q_{HH}(v)$ is symmetric, orthogonal and has determinant -1.

It can be shown that any d-dimensional orthogonal matrix Q can be represented as the product of at most d Householder reflection matrices. The two-dimensional generator $G(\theta)$ is recovered as the Householder matrix $Q_{HH}(v)$ with $v = \begin{pmatrix} -\sin\frac{\theta}{2} \\ \cos\frac{\theta}{2} \end{pmatrix}$ or $v = \begin{pmatrix} \sin\frac{\theta}{2} \\ -\cos\frac{\theta}{2} \end{pmatrix}$.

Permutation matrix

A special type of an orthogonal matrix is a permutation matrix P created by permuting rows and/or columns of the identity matrix I. Thus, each row and column of P contains exactly one entry of 1, but not necessarily on the diagonal.

If a permutation matrix P is multiplied with a matrix A it acts as an operator permuting the columns (AP) or the rows (PA). For a set of d elements there exist $d!$ permutations. Thus, for dimension d there are $d!$ possible permutation matrices (including the identity matrix).

The determinant of a permutation matrix is either +1 or -1. The product of two permutation matrices yields another permutation matrix.

Symmetric permutation matrices correspond to self-inverse permutations (i.e. the permutation matrix is its own inverse), and are also called permutation involutions. They can have determinant +1 and -1.

A transposition is a permutation where only two elements are exchanged. Thus, in a transposition matrix T exactly two rows and/or columns are exchanged compared to identity matrix I. Transpositions are self-inverse, and transposition matrices are symmetric. There are $\frac{d(d-1)}{2}$ different transposition matrices. The determinant of a transposition matrix is $\det(T) = -1$.

Note that the transposition matrix is an instance of a Householder matrix $Q_{HH}(v)$ with vector v filled with zeros except for two elements that have value $\frac{\sqrt{2}}{2}$ and $-\frac{\sqrt{2}}{2}$.

Any permutation of d elements can be generated by a series of at most $d-1$ transpositions. Correspondingly, any permutation matrix P can be constructed by multiplication of the identity matrix with at most $d-1$ transposition matrices. If the number of transpositions is even then

$\det(P) = 1$ otherwise for an uneven number $\det(P) = -1$. This is called the sign or signature of the permutation.

The set of all permutations form the symmetric group S_d, the subset of even permutations (with positive sign and $\det(P) = 1$) the alternating group A_d.

1.7 Eigenvalues and eigenvectors

Definition

Assume a square matrix A of size $d \times d$. A vector $u \neq 0$ is called an eigenvector of the matrix A and λ the corresponding eigenvalue if

$$A u = u \lambda \,.$$

This is called **eigenvalue equation** or **eigenequation**.

Finding eigenvalues and vectors

To find the eigenvalues and eigenvectors the eigenequation is rewritten as

$$(A - I\lambda)\, u = 0 \,.$$

For this equation to hold for an eigenvector $u \neq 0$ with eigenvalue λ implies that the matrix $A - I\lambda$ is singular. Correspondingly, its determinant must vanish

$$\det(A - I\lambda) = 0 \,.$$

This is called the *characteristic equation* of the matrix A, and its solution yields the d eigenvalues $\lambda_1, \ldots, \lambda_d$. Note the eigenvalues need not be distinct and they may be complex even if the matrix A is real.

If there are complex eigenvalues, for a real matrix those eigenvalues come in conjugate pairs. Hence, for a complex $\lambda_1 = re^{i\phi}$ there will also be a corresponding complex eigenvalue $\lambda_2 = re^{-i\phi}$.

Given the eigenvalues we then solve the eigenequation for the corresponding non-zero eigenvectors $u_1, \ldots, u_d$. Note that eigenvectors of real matrices can have complex components. Also the eigenvector is only defined by the eigenequation up to a scalar. By convention eigenvectors are therefore typically standardised to unit length but this still

leaves a sign ambiguity for real eigenvectors and implies that complex eigenvectors are defined only up to a factor with modulus 1.

Eigenequation in matrix notation

With the matrix
$$U = (u_1, \ldots, u_d)$$
containing the standardised eigenvectors in the columns and the diagonal matrix
$$\Lambda = \begin{pmatrix} \lambda_1 & \ldots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \ldots & \lambda_d \end{pmatrix}$$
containing the eigenvalues (typically sorted in order of magnitude) the eigenvalue equation can be written as
$$AU = U\Lambda.$$

Permutation of eigenvalues

If eigenvalues are not in order, we may apply a permutation matrix P to arrange them in order. With $\Lambda^{\text{sort}} = P^T \Lambda P$ as the sorted eigenvalues and $U^{\text{sort}} = UP$ as the corresponding eigenvectors the eigenequation becomes
$$AU^{\text{sort}} = AUP = U\Lambda P = UPP^T \Lambda P = U^{\text{sort}}\Lambda^{\text{sort}}.$$

Similar matrices

Two matrices A and B are called **similar** if they share the same eigenvalues.

From A with eigenvalues Λ and eigenvectors U we can construct a similar B via the **similarity transformation** $B = MAM^{-1}$ where M is an invertible matrix.

Then Λ are the eigenvalues of B and $V = MU$ its eigenvectors as
$$BV = MAM^{-1}MU = MAU = MU\Lambda = V\Lambda.$$

Defective matrix

In most cases the eigenvectors u_i will be linearly independent so that they form a basis to span a d dimensional space.

However, if this is not the case and the matrix A does not have a complete basis of eigenvectors, then the matrix is called defective. In this case the matrix U containing the eigenvectors is singular and $\det(U) = 0$.

An example of a defective matrix is $\begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix}$ which has determinant 1 so that it can be inverted and its column vectors do form a complete basis but has only one distinct eigenvector $(1,0)^T$ so that the eigenvector basis is incomplete.

Eigenvalues of a diagonal or triangular matrix

In the special case that A is diagonal or a triangular matrix the eigenvalues are easily determined. This follows from the simple form of their determinants as the product of the diagonal elements. Hence for these matrices the characteristic equation becomes $\prod_i^d (a_{ii} - \lambda) = 0$ and has solution $\lambda_i = a_{ii}$, i.e. the eigenvalues are equal to the diagonal elements.

Eigenvalues and vectors of a symmetric matrix

If A is symmetric, i.e. $A = A^T$, then its eigenvalues and eigenvectors have special properties:

  i) all eigenvalues of A are real,
 ii) the eigenvectors are orthogonal, i.e $u_i^T u_j = 0$ for $i \neq j$, and real. Thus, the matrix U containing the standardised orthonormal eigenvectors is orthogonal.
iii) A is never defective as U forms a complete basis.

Furthermore, for a symmetric matrix A with diagonal elements $p_1 \geq \ldots \geq p_d$ and eigenvalues $\lambda_1 \geq \ldots \geq \lambda_d$ (note both written in decreasing order) the sum of the largest k eigenvalues forms an upper bound of the sum of the largest k diagonal elements:

$$\sum_i^k \lambda_i \geq \sum_i^k p_i$$

This theorem is due to Schur (1923) [2]. The equality holds for $k = d$ (as the trace of A equals the sum of its eigenvalues) and for any k if A is diagonal (as in this case of the diagonal elements equal the eigenvalues).

Eigenvalues of orthogonal matrices

The eigenvalues of an orthogonal matrix Q are not necessarily real but they all have modulus 1 and lie on the unit circle . Thus, the eigenvalues of Q all have the form $\lambda = e^{i\phi} = \cos\phi + i\sin\phi$.

In any real matrix complex eigenvalues come in conjugate pairs. Hence if an orthogonal matrix Q has the complex eigenvalue $e^{i\phi}$ it also has an complex eigenvalue $e^{-i\phi} = \cos\phi - i\sin\phi$. The product of these two conjugate eigenvalues is 1. Thus, an orthogonal matrix of uneven dimension has at least one real eigenvalue (+1 or -1).

The eigenvalues of a Hausholder matrix $Q_{HH}(v)$ are all real (recall that it is symmetric!). In fact, in dimension d its eigenvalues are -1 (one time) and 1 ($d - 1$ times). Since a transposition matrix T is a special Householder matrix they have the same eigenvalues.

Positive definite matrices

If all eigenvalues of a square matrix A are real and $\lambda_i \geq 0$ then A is called *positive semi-definite*. If all eigenvalues are strictly positive $\lambda_i > 0$ then A is called *positive definite*.

Note that a matrix does not need to be symmetric to be positive definite, e.g. $\begin{pmatrix} 2 & 3 \\ 1 & 4 \end{pmatrix}$ has positive eigenvalues 5 and 1. It also has a complete set of eigenvectors and is diagonalisable.

A symmetric matrix A is positive definite if the quadratic form $x^T A x > 0$ for any non-zero x, and it is positive semi-definite if $x^T A x \geq 0$. This holds also the other way around: a symmetric positive definite matrix (with positive eigenvalues) has a positive quadratic form, and a symmetric positive semi-definite matrix (with non-negative eigenvalues) a non-negative quadratic form.

A symmetric positive definite matrix always has a positive diagonal (this can be seen by setting x above to a unit vector with 1 at a single position,

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[2]Schur, I. 1923. Über eine Klasse von Mittelbildungen mit Anwendungen auf die Determinantentheorie. Sitzungsber. Berl. Math. Ges. **22**:9–29.

and 0 at all other elements). However, just requiring a positive diagonal is too weak to ensure positive definiteness of a symmetric matrix, for example $\begin{pmatrix} 1 & 10 \\ 10 & 1 \end{pmatrix}$ has a negative eigenvalue of -9. On the other hand, a symmetric matrix is indeed positive definite if it is strictly diagonally dominant, i.e. if all its diagonal elements are positive and are larger than the absolute value of any of the corresponding row or column elements. However, diagonal dominance is too restrictive as criterion to characterise all symmetric positive definite matrices, since there are many symmetric matrices that are positive definite but not diagonally dominant, such as $\begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix}$.

Finally, the sum of a symmetric positive semi-definite matrix A and a symmetric positive definite matrix B is itself symmetric positive definite because the corresponding quadratic form $x^T(A+B)x = x^T Ax + x^T Bx > 0$ is positive. Similarly, the sum of two symmetric positive (semi)-definite matrices is itself symmetric positive (semi)-definite.

1.8 Matrix decompositions

Diagonalisation and eigenvalue decomposition

If A is a square non-defective matrix then the eigensystem U is invertible and we can rewrite the eigenvalue equation to

$$A = U\Lambda U^{-1}.$$

This is called the **eigendecomposition**, or **spectral decomposition**, of A and equivalently

$$\Lambda = U^{-1}AU$$

is the diagonalisation of A.

If A is defective (i.e. U is singular) one can still *approximately* diagonalise A as there always exists a similarity transformation to $J = MAM^{-1}$ where M is a invertible matrix and J has Jordan canonical form, i.e. J is upper triangular with the (potentially complex) eigenvalues on the diagonal and some non-zero entries equal to 1 immediately above the main diagonal.

Orthogonal eigenvalue decomposition

For symmetric A with real eigenvalues and orthogonal matrix U the spectral decomposition becomes

$$A = U\Lambda U^T$$

and

$$\Lambda = U^T A U .$$

This special case is known as the orthogonal diagonalisation of A.

The orthogonal decomposition for symmetric A is unique apart from the signs of the eigenvectors (columns of U). Thus, in a computer application depending on the specific implementation of a numerical algorithm for eigenvalue decomposition the signs may vary.

Singular value decomposition

The **singular value decomposition** (SVD) is a generalisation of the orthogonal eigenvalue decomposition for symmetric matrices.

Any (!) rectangular matrix A of size $n \times d$ can be factored into the product

$$A = U D V^T$$

where U is a $n \times n$ orthogonal matrix, V is a second $d \times d$ orthogonal matrix and D is a diagonal but rectangular matrix of size $n \times d$ with $m = min(n, d)$ real diagonal elements $d_1, \ldots d_m$. The d_i are called singular values, and appear along the diagonal in D by order of magnitude.

The SVD is unique apart from the signs of the columns vectors in U, V and D (you can freely specify the column signs of any two of the three matrices). By convention the signs are chosen such that the singular values in D are all non-negative, which leaves ambiguity in columns signs of U and V. Alternatively, one may fix the columns signs of U and V, e.g. by requiring a positive diagonal, which then determines the sign of the singular values (thus allowing for negative singular values as well).

If A is symmetric then the SVD and the orthogonal eigenvalue decomposition coincide (apart from different sign conventions for singular values, eigenvalues and eigenvectors).

Since $A^T A = V D^T D V^T$ and $A A^T = U D D^T U^T$ the squared singular values correspond to the eigenvalues of $A^T A$ and $A A^T$. It also follows

that $A^T A$ and AA^T are both positive semi-definite symmetric matrices, and that V and U contain the respective sets of eigenvectors.

Polar decomposition

Any square matrix A can be factored into the product

$$A = QB$$

of an orthogonal matrix Q and a symmetric positive semi-definite matrix B.

This follows from the SVD of A given as

$$\begin{aligned}
A &= UDV^T \\
&= (UV^T)(VDV^T) \\
&= QB
\end{aligned}$$

with non-negative D. Note that this decomposition is unique as the sign ambiguities in the columns of U and V cancel out in Q and B.

Cholesky decomposition

A symmetric positive definite matrix A can be decomposed into a product of a triangular matrix L with its transpose

$$A = LL^T .$$

Here, L is a lower triangular matrix with positive diagonal elements.

This decomposition is unique and is called **Cholesky factorisation**. It is often used to check whether a symmetric matrix is positive definite as it is algorithmically less demanding than eigenvalue decomposition.

Note that some implementations of the Cholesky decomposition (e.g. in R) use upper triangular matrices K with positive diagonal so that $A = K^T K$ and $L = K^T$.

1.9 Matrix summaries based on eigenvalues and singular values

Trace and determinant computed from eigenvalues

The eigendecomposition $A = U\Lambda U^{-1}$ allows to establish a link between the trace and the determinant and the eigenvalues of a matrix.

Specifically,

$$\mathrm{Tr}(A) = \mathrm{Tr}(U\Lambda U^{-1}) = \mathrm{Tr}(\Lambda U^{-1}U)$$

$$= \mathrm{Tr}(\Lambda) = \sum_{i=1}^{d} \lambda_i$$

thus the trace of a square matrix A is equal to the *sum* of its eigenvalues. Likewise,

$$\det(A) = \det(U)\det(\Lambda)\det(U^{-1})$$

$$= \det(\Lambda) = \prod_{i=1}^{d} \lambda_i$$

therefore the determinant of A is the *product* of the eigenvalues.

The relationship between the eigenvalues of a square matrix and the trace and the determinant of that matrix is shown above for diagonalisable matrices. However, it holds more generally for any square matrix, i.e. also for defective matrices. For the latter the Jordan canonical form J replaces Λ (in both cases the eigenvalues are simply the entries on the diagonal).

If any of the eigenvalues are equal to zero then $\det(A) = 0$ and as hence A is singular and not invertible.

The trace and determinant of a real matrix are always real even though the individual eigenvalues may be complex.

Eigenvalues of a squared matrix

From the eigendecomposition $A = U\Lambda U^{-1}$ it is easy to see that the eigenvalues of A^2 are simply the squared eigenvalues of A as

$$A^2 = U\Lambda U^{-1}U\Lambda U^{-1} = U\Lambda^2 U^{-1}$$

As a result we can compute the trace of A^2 as the sum of the squared eigenvalues of A, i.e. $\text{Tr}(A^2) = \sum_{i=1}^{d} \lambda_i^2$, and the determinant as the product of squared eigenvalues, i.e $\det(A^2) = \prod_{i=1}^{d} \lambda_i^2$.

If A is symmetric then $\text{Tr}(A^2) = \text{Tr}(AA^T) = ||A||_F^2 = \sum_{i=1}^{d} \sum_{j=1}^{d} a_{ij}^2$. This leads to the identity

$$\sum_{i=1}^{d} \lambda_i^2 = \sum_{i=1}^{d} \sum_{j=1}^{d} a_{ij}^2$$

between the sum of the squared eigenvalues and the sum of all squared entries of a symmetric matrix A.

Rank and condition number

The rank is the dimension of the space spanned by both the column and row vectors. A rectangular matrix of dimension $n \times d$ will have rank of at most $m = \min(n, d)$, and if the maximum is indeed achieved then it has full rank.

The condition number describes how well- or ill-conditioned a full rank matrix is. For example, for a square matrix a large condition number implies that the matrix is close to being singular and thus ill-conditioned. If the condition number is infinite then the matrix is not full rank.

The rank and condition of a matrix can both be determined from the m singular values $d_1, \ldots, d_m$ of a matrix obtained by SVD:

i) The rank is number of non-zero singular values.
ii) The condition number is the ratio of the largest singular value divided by the smallest singular value (absolute values if signs are allowed).

If a square matrix A is singular then the condition number is infinite, and it will not have full rank. On the other hand, a non-singular square matrix, such as a positive definite matrix, has full rank.

1.10 Functions of symmetric matrices

We focus on *symmetric* square matrices $A = U \Lambda U^T$ which are always diagonalisable with real eigenvalues Λ and orthogonal eigenvectors U.

Definition of a matrix function

Assume a real-valued function $f(a)$ of a real number a. Then the corresponding matrix function $f(A)$ is defined as

$$f(A) = U f(\Lambda) U^T = U \begin{pmatrix} f(\lambda_1) & \cdots & 0 \\ \vdots & \ddots & \vdots \\ 0 & \cdots & f(\lambda_d) \end{pmatrix} U^T$$

where the function $f(a)$ is applied to the eigenvalues of A. By construction $f(A)$ is real, symmetric and has real eigenvalues $f(\lambda_i)$.

Examples:

Example 1.2. Matrix power: $f(a) = a^p$ (with p a real number)

Special cases of matrix power include :

- Matrix inversion: $f(a) = a^{-1}$
  Note that if the matrix A is singular, i.e. contains one or more eigenvalues $\lambda_i = 0$, then A^{-1} is not defined and therefore A is not invertible.

However, a so-called *pseudoinverse* can still be computed, by inverting the non-zero eigenvalues, and keeping the zero eigenvalues as zero.

- Matrix square root: $f(a) = a^{1/2}$
  Since there are multiple solutions to the square root there are also multiple matrix square roots. The principal matrix square root is obtained by using the positive square roots of all the eigenvalues. Thus the **principal matrix square root** of a positive semi-definite matrix is also positive semi-definite and it is unique.

Example 1.3. Matrix exponential: $f(a) = \exp(a)$
Note that because $\exp(a) \geq 0$ for all real a the matrix $\exp(A)$ is positive semi-definite. Thus, the matrix exponential can be used to generate positive semi-definite matrices.

If A and B commute, i.e. if $AB = BA$, then $\exp(A + B) = \exp(A)\exp(B)$. However, this is not the case otherwise!

Example 1.4. Matrix logarithm: $f(a) = \log(a)$
As the logarithm requires $a > 0$ the matrix A needs to be positive definite for $\log(A)$ to be defined.

Identities for the matrix exponential and logarithm

The above give rise to useful identities:

1) For any symmetric matrix A we have

$$\det(\exp(A)) = \exp(\mathrm{Tr}(A))$$

because $\prod_i \exp(\lambda_i) = \exp(\sum_i \lambda_i)$ where λ_i are the eigenvalues of A.

2) If we take the logarithm on both sides and replace $\exp(A) = B$ we get another identity for a symmetric positive definite matrix B:

$$\log \det(B) = \mathrm{Tr}(\log(B))$$

because $\log(\prod_i \lambda_i) = \sum_i \log(\lambda_i)$ where λ_i are the eigenvalues of B.

2 Vector and matrix calculus

2.1 First order vector derivatives

Derivative and gradient

The **derivative** of a scalar-valued function $h(x)$ with regard to its vector argument $x = (x_1, \ldots, x_d)^T$ is the *row vector*

$$Dh(x) = \frac{\partial h(x)}{\partial x} = \left(\frac{\partial h(x)}{\partial x_1} \quad \cdots \quad \frac{\partial h(x)}{\partial x_d} \right)$$

The above notation follows the **numerator layout** convention, where the dimension of the numerator (here 1) determines the number of rows and the dimension of the denominator (here d) the number of columns of the resulting matrix (see https://en.wikipedia.org/wiki/Matrix_calculus for details). For a scalar function this results in a vector of the same dimension as x^T.

The **gradient** of $h(x)$ is a *column vector* and the transpose of the derivative

$$\text{grad } h(x) = \left(\frac{\partial h(x)}{\partial x} \right)^T$$

It is often written using the **nabla operator** ∇ as

$$\nabla h(x) = \begin{pmatrix} \frac{\partial h(x)}{\partial x_1} \\ \vdots \\ \frac{\partial h(x)}{\partial x_d} \end{pmatrix}$$

with

$$\nabla = \begin{pmatrix} \frac{\partial}{\partial x_1} \\ \vdots \\ \frac{\partial}{\partial x_d} \end{pmatrix}$$

Note that
$$(\nabla h(x))^T = \nabla^T h(x) = Dh(x) = \frac{\partial h(x)}{\partial x}$$

Example 2.1. Examples for the gradient and derivative:

- $h(x) = a^T x + b$.
  Then $\nabla h(x) = a$ and $Dh(x) = \frac{\partial h(x)}{\partial x} = a^T$.
- $h(x) = x^T x$.
  Then $\nabla h(x) = 2x$ and $Dh(x) = \frac{\partial h(x)}{\partial x} = 2x^T$.
- $h(x) = x^T A x$.
  Then $\nabla h(x) = (A + A^T)x$ and $Dh(x) = \frac{\partial h(x)}{\partial x} = x^T(A + A^T)$.

Jacobian matrix

Similarly, we can also compute the **derivative** of a vector-valued function
$$h(x) = (h_1(x), \dots, h_m(x))^T$$

with regard to x. This yields (again in numerator layout convention) a matrix of size m rows and d columns whose rows contain the derivatives of the components of $h(x)$.

$$Dh(x) = \frac{\partial h(x)}{\partial x} = \left(\frac{\partial h_i(x)}{\partial x_j}\right)$$

$$= \begin{pmatrix} \frac{\partial h_1(x)}{\partial x_1} & \cdots & \frac{\partial h_1(x)}{\partial x_d} \\ \vdots & \ddots & \vdots \\ \frac{\partial h_m(x)}{\partial x_1} & \cdots & \frac{\partial h_m(x)}{\partial x_d} \end{pmatrix}$$

$$= \begin{pmatrix} \nabla^T h_1(x) \\ \vdots \\ \nabla^T h_m(x) \end{pmatrix}$$

This matrix is also called the **Jacobian matrix**

Example 2.2. $h(x) = A^T x + b$. Then $Dh(x) = \frac{\partial h(x)}{\partial x} = A^T$.

If $m = d$ then the Jacobian matrix is a square and this allows to compute the **determinant of the Jacobian matrix**. Both the Jacobian matrix and the Jacobian determinant are often called "the Jacobian" so one needs

to determine from the context whether this refers to the matrix or the determinant.

If $y = h(x)$ is an invertible function with $x = h^{-1}(y)$ then the Jacobian matrix is invertible and the inverted matrix is the Jacobian matrix of the inverse function:

$$Dx(y) = \left(Dy(x)\right)^{-1}|_{x=x(y)}$$

or in alternative notation

$$\frac{\partial x(y)}{\partial y} = \left(\frac{\partial y(x)}{\partial x}\right)^{-1}\Bigg|_{x=x(y)}$$

In this case the Jacobian determinant of the back-transformation can be computed as the inverse of the Jacobian determinant of the original function:

$$\det Dx(y) = \det \left(Dy(x)\right)^{-1}|_{x=x(y)}$$

and

$$\det \left(\frac{\partial x(y)}{\partial y}\right) = \det \left(\frac{\partial y(x)}{\partial x}\right)^{-1}\Bigg|_{x=x(y)}$$

2.2 Second order vector derivatives

The matrix of all second order partial derivates of scalar-valued function with vector-valued argument is called the **Hessian matrix**:

$$\nabla\nabla^T h(x) = \begin{pmatrix} \frac{\partial^2 h(x)}{\partial x_1^2} & \frac{\partial^2 h(x)}{\partial x_1\partial x_2} & \cdots & \frac{\partial^2 h(x)}{\partial x_1\partial x_d} \\ \frac{\partial^2 h(x)}{\partial x_2\partial x_1} & \frac{\partial^2 h(x)}{\partial x_2^2} & \cdots & \frac{\partial^2 h(x)}{\partial x_2\partial x_d} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial^2 h(x)}{\partial x_d\partial x_1} & \frac{\partial^2 h(x)}{\partial x_d\partial x_2} & \cdots & \frac{\partial^2 h(x)}{\partial x_d^2} \end{pmatrix}$$

$$= \left(\frac{\partial h(x)}{\partial x_i\partial x_j}\right)$$

$$= \frac{\partial}{\partial x}\left(\frac{\partial h(x)}{\partial x}\right)^T$$

$$= D(Dh(x))^T$$

By construction the Hessian matrix is square and symmetric.

Example 2.3. $h(x) = x^T Ax$. Then $\nabla\nabla^T h(x) = (A + A^T)$.

2.3 Chain rules for gradient vector and Hessian matrix

Suppose $h(x)$ is a scalar-valued function and $g(y) = h(x(y))$ is a composite scalar-valued function where $x(y)$ a map from y to x.

The gradient of the composite function $g(y) = h(x(y))$ can be computed from the gradient of $h(x)$ and the Jacobian matrix for $x(y)$ as follows:

$$\nabla g(y) = (Dx(y))^T \nabla h(x)|_{x=x(y)}$$

and

$$\nabla g(y) = \left(\frac{\partial x(y)}{\partial y}\right)^T \nabla h(x)|_{x=x(y)}$$

Similarly, the Hessian matrix of $g(y)$ can be computed from the Hessian of $h(x)$ and the Jacobian matrix for $x(y)$:

$$\nabla \nabla^T g(y) = (Dx(y))^T \nabla \nabla^T h(x)|_{x=x(y)} Dx(y)$$

and

$$\nabla \nabla^T g(y) = \left(\frac{\partial x(y)}{\partial y}\right)^T \nabla \nabla^T h(x)|_{x=x(y)} \frac{\partial x(y)}{\partial y}$$

2.4 First order matrix derivatives

The derivative of a scalar-valued function $h(X)$ with regard to a matrix argument $X = (x_{ij})$ is defined as below and and results (in numerator layout convention) in a matrix of the same dimension as X^T:

$$Dh(X) = \frac{\partial h(X)}{\partial X} = \left(\frac{\partial h(X)}{\partial x_{ji}}\right)$$

Example 2.4. Examples for first order matrix derivatives:

- $\frac{\partial \operatorname{Tr}(A^T X)}{\partial X} = A^T$
- $\frac{\partial \operatorname{Tr}(A^T XB)}{\partial X} = BA^T$
- $\frac{\partial \operatorname{Tr}(X^T AX)}{\partial X} = X^T(A + A^T)$
- $\frac{\partial \log \det(X)}{\partial X} = \frac{\partial \operatorname{Tr}(\log X)}{\partial X} = X^{-1}$

2.5 **Linear and quadratic approximation**

A linear and quadratic approximation of a differentiable function is given by a Taylor series of first and second order, respectively.

i) Linear and quadratic approximation of a scalar-valued function of a scalar:

$$h(x) \approx h(x_0) + h'(x_0)(x - x_0) + \frac{1}{2}h''(x_0)(x - x_0)^2$$

Note that $h'(x_0) = h'(x)| x_0$ is first derivative of $h(x)$ evaluated at x_0 and $h''(x_0) = h''(x)| x_0$ is the second derivative of $h(x)$ evaluated x_0.

With $x = x_0 + \varepsilon$ the approximation can also be written as

$$h(x_0 + \varepsilon) \approx h(x_0) + h'(x_0)\varepsilon + \frac{1}{2}h''(x_0)\varepsilon^2$$

The first two terms on the right comprise the linear approximation, all three terms the quadratic approximation.

ii) Linear and quadratic approximation of a scalar-valued function of a vector:

$$h(x) \approx h(x_0) + \nabla^T h(x_0)(x - x_0) + \frac{1}{2}(x - x_0)^T \nabla\nabla^T h(x_0)(x - x_0)$$

Note that $\nabla^T h(x_0)$ is the transposed gradient (i.e the vector derivative) of $h(x)$ evaluated at x_0 and $\nabla\nabla^T h(x_0)$ the Hessian matrix of $h(x)$ evaluated at x_0. With $x = x_0 + \varepsilon$ this approximation can also be written as

$$h(x_0 + \varepsilon) \approx h(x_0) + \nabla^T h(x_0)\varepsilon + \frac{1}{2}\varepsilon^T \nabla\nabla^T h(x_0)\varepsilon$$

The first two terms on the right comprise the linear approximation, all three terms the quadratic approximation.

iii) Linear approximation of a vector-valued function of a vector:

$$h(x) \approx h(x_0) + Dh(x_0)(x - x_0)$$

Note that $Dh(x_0)$ is Jacobian matrix (i.e the vector derivative) of $h(x)$ evaluated at x_0. With $x = x_0 + \varepsilon$ this approximation can also be written as

$$h(x_0 + \varepsilon) \approx h(x_0) + Dh(x_0)\varepsilon$$

Example 2.5. Examples of Taylor series approximations of second order:

- $\log(x_0 + \varepsilon) \approx \log(x_0) + \frac{\varepsilon}{x_0} - \frac{\varepsilon^2}{2x_0^2}$
- $\frac{x_0}{x_0 + \varepsilon} \approx 1 - \frac{\varepsilon}{x_0} + \frac{\varepsilon^2}{x_0^2}$

Example 2.6. Around a local extremum x_0 (maximum or minimum) where the gradient vanishes ($h(x_0) = 0$) the quadratic approximation of the function $h(x)$ simplifies to

$$h(x_0 + \varepsilon) \approx h(x_0) + \frac{1}{2}\varepsilon^T \nabla\nabla^T h(x_0)\varepsilon$$

2.6 Conditions for a local extremum of a function

To check if x_0 or x_0 is a local extremum, i.e. a local maximum or a local minimum, of a differentiable function $h(x)$ or $h(x)$ we can use the following conditions:

For a function of a single variable:

- i) First derivative is zero at the extremum: $h'(x_0) = 0$.
- ii) If the second derivative $h''(x_0) < 0$ at the extremum is negative then it is a maximum.
- iii) If the second derivative $h''(x_0) > 0$ at the extremum is positive it is a minimum.

Note that conditions ii) and iii) are sufficient but not necessary. For a minimum, it is necessary that the second derivative is non-negative, and for a maximum that the second derivative is non-positive.

For a function of several variables:

- i) Gradient vanishes at extremum: $\nabla h(x_0) = 0$.
- ii) If the Hessian $\nabla\nabla^T h(x_0)$ is negative definite (= all eigenvalues of Hessian matrix are negative) then the extremum is a maximum.
- iii) If the Hessian is positive definite (= all eigenvalues of Hessian matrix are positive) then the extremum is a minimum.

Again, conditions ii) and iii) are sufficient but not necessary. For a minimum it is necessary that the Hessian is positive semi-definite, and for a maximum that the Hessian is negative semi-definite.

Example 2.7. Minimum with vanishing second derivative:

x^4 clearly has a minimum at $x_0 = 0$. As required the first derivative $4x^3$ vanishes at $x_0 = 0$. However, the second derivative $12x^2$ also vanishes at $x_0 = 0$, showing that a positive second derivative is not necessary for a minimum.

2.7 Convex and concave functions

A function $h(x)$ is **convex** if for all x_1 and x_2 the line segment from point $(x_1, h(x_1))$ to point $(x_2, h(x_2))$ never lies below the function. Moreover, the function is strictly convex if the line segment always lies above the curve, apart from the two end points:

$$\lambda h(x_1) + (1 - \lambda)h(x_2) \geq h(\lambda x_1 + (1 - \lambda)x_2)$$

for all $\lambda \in [0, 1]$.

Equivalently, a differentiable function $h(x)$ is convex (strictly convex) if for all x_0 the function $h(x)$ never lies below (always lies above, except at x_0) the linear approximation through the point $(x_0, h(x_0))$:

$$h(x) \geq h(x_0) + \nabla^T h(x_0)(x - x_0)$$

For a convex function a vanishing gradient at x_0 indicates a minimum at x_0. Furthermore, any local minimum must also be a global minimum (for a differentiable function this follows directly from the last inequality). For a strictly convex function the minimum is unique so there is at most one local/global minimum in that case.

If $h(x)$ is convex, then $-h(x)$ is **concave**, and the criteria above can be adapted accordingly to check for concavity and strict concavity, as well as to identify local/global maxima.

(Strictly) convex and concave functions are convenient objective functions in optimisation as it is straightforward to find their local/global extrema, both analytically and numerically.

As the shape of a convex function resembles that of a valley, one way to memorise that fact is that a **va**lley is con**ve**x.

Example 2.8. Convex functions:

This is a convex function but not a strictly convex function:

- $\max(x^2, |x|)$

The following are strictly convex functions:

- x^2,
- x^4,
- e^x,
- $x \log(x)$ for $x > 0$.

On the other hand, this is not a convex function:

- $\frac{1}{x^2}$ for all $x \neq 0$.

However, the function in last example is strictly convex if the domain is restricted to either $x > 0$ or $x < 0$.

Example 2.9. Concave functions:

The following are strictly concave functions:

- $-x^2$,
- $\log(x)$ for $x > 0$,
- $\sqrt{x}$ for $x > 0$.