Foundations
for complex systems modeling

Abstract. These lecture notes are largely based on a previous version prepared by A. Annibale, B. Bravi, N. Shayeghi, and M. Poplavskyi for a 7-lectures *Foundations* course at King's College London. The notes have been reviewed, rearranged and re-edited by G. Sicuro in 2021. The purpose of the notes is to give a fast and compact review of elementary mathematical tools and results useful for the MSc in Complex System Modelling at King's College London. As general rich reference (amongst many possibility) we recommend the book by Arfken, Weber and Harris, *Mathematical Methods for Physicists: A Comprehensive Guide* published in 2012 by Academic Press, or the book *Mathematics for Physicists* by Philippe Dennery and André Krzywicki, published by Dover.

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LECTURE 1

Linear Algebra

1. Matrix and vector operations

The first building block to construct a matrix is some *field* $\mathbb{F}$. A field is defined as follows.

DEFINITION 1.1. *A field is a set* $\mathbb{F}$ *endowed with two binary operations, a multiplication* $\cdot$ *and an addition* $+$*. Both this operations map an ordered pair of element of* $\mathbb{F}$ *to another element of* $\mathbb{F}$*,* $\mathbb{F} \times \mathbb{F} \to \mathbb{F}$*. These two operations have to satisfy the following properties for each triplet* $a, b, c \in \mathbb{F}$*:*

Associativity: *For both* $\circ = +$ *and* $\circ = \cdot$*, then* $a \circ (b \circ c) = (a \circ b) \circ c$*.*

Commutativity: *For both* $\circ = +$ *and* $\circ = \cdot$*, then* $a \circ b = b \circ a$*.*

Existence of identities: *There exists two special element in* $\mathbb{F}$*, zero, denoted by* 0*, and one, denoted by* 1*, such that* $a + 0 = a$ *and* $a \cdot 1 = a$*.*

Inverse: *For each* $a \in \mathbb{F}$ *there is an element, denoted by* $-a \in \mathbb{F}$*, such that* $a + (-a) = 0$*. Similarly, for each* $a \in \mathbb{F} \setminus \{0\}$ *there is an element* $1/a \in \mathbb{F}$ *such that* $a \cdot 1/a = 1$*.*

Distributivity of $\cdot$ over $+$: $a \cdot (b + c) = a \cdot b + a \cdot c$*.*

In the following we will often omit $\cdot$ in writing down the multiplication. The abstract definition of field includes some sets of numbers we are familiar with, e.g., the set of rational numbers $\mathbb{Q}$, the set of real numbers $\mathbb{R}$ and the set of complex numbers $\mathbb{C}$ (notably, not the set of integer numbers $\mathbb{Z}$). Once a field is given, a *matrix* can be defined as an array of elements of such field.

DEFINITION 1.2. *A matrix* $\boldsymbol{A}$ *is an* $n \times m$ *array of entries* $A_{ij} \equiv [\boldsymbol{A}]_{ij}$ *from a given field* $\mathbb{F}$*, with* $i = 1, \dots, n$ *and* $j = 1, \dots, m$*. We denote by* $\mathcal{M}_{n\times m}(\mathbb{F})$ *the set of all such matrices. If dimensions of a matrix are equal, the matrix is called square. A square matrix* $\boldsymbol{A}$ *is called diagonal if* $A_{ij} = 0$ *for* $i \neq j$*. A diagonal matrix of size* n *with ones on a diagonal is denoted by* $\boldsymbol{I}_n$ *and called identity matrix.*

Given $\boldsymbol{A} \in \mathcal{M}_{n\times m}(\mathbb{F})$, we call introduce the *transpose* matrix $\boldsymbol{A}^\top \in \mathcal{M}_{m\times n}(\mathbb{F})$, such that $[\boldsymbol{A}^\top]_{ij} = A_{ji}$. A square matrix $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{F})$ is *symmetric* if $\boldsymbol{A} = \boldsymbol{A}^\top$. In particular, if $\mathbb{F} = \mathbb{R}$ a symmetric matrix is sometimes called *real symmetric*. If $\mathbb{R} = \mathbb{C}$, a special class of matrix is the family of *Hermitian matrices*, i.e., matrices $\boldsymbol{A}$ such that $\boldsymbol{A} = \boldsymbol{A}^\dagger$, where $\boldsymbol{A}^\dagger$ is the *Hermitian transpose* matrix obtained from $\boldsymbol{A}$ taking the transpose and the complex conjugation of all its elements. Note that an Hermitian matrix with real entries is a real symmetric matrix.

Below we call a *vector* $\boldsymbol{v} \in \mathcal{M}_{n\times 1}(\mathbb{F}) \equiv \mathbb{F}^n$ a matrix of dimension $n \times 1$ (i.e., a "column" of n rows).

Given two matrices $\boldsymbol{A}, \boldsymbol{B} \in \mathcal{M}_{n\times m}(\mathbb{F})$, the sum $\boldsymbol{C} = \boldsymbol{A} + \boldsymbol{B}$ of matrices is defined as an element-wise operation

$$C_{ij} = A_{ij} + B_{ij} \tag{1}$$

The product is instead defined as an operation $\mathcal{M}_{n\times m}(\mathbb{F})\times\mathcal{M}_{m\times n'}(\mathbb{F}) \to \mathcal{M}_{n\times n'}(\mathbb{F})$ so that

$$\boldsymbol{C} = \boldsymbol{AB} \Leftrightarrow C_{ij} = \sum_{k=1}^{m} A_{ik}B_{kj}. \tag{2}$$

Observe that if $\boldsymbol{C} = \boldsymbol{AB}$, the matrix $\boldsymbol{BA}$ is not defined unless $\boldsymbol{A}$ and $\boldsymbol{B}$ are both squared of the same dimension. Even in this case, however, $\boldsymbol{AB} \neq \boldsymbol{BA}$ in general. For example if $\boldsymbol{A} = \left(\begin{smallmatrix} 1 & 0 \\ 1 & 1 \end{smallmatrix}\right)$ and $\boldsymbol{B} = \left(\begin{smallmatrix} 1 & 1 \\ 0 & 1 \end{smallmatrix}\right)$, then $\boldsymbol{AB} = \left(\begin{smallmatrix} 1 & 1 \\ 1 & 2 \end{smallmatrix}\right)$ but $\boldsymbol{BA} = \left(\begin{smallmatrix} 2 & 1 \\ 1 & 1 \end{smallmatrix}\right)$. Finally, for any matrix $\boldsymbol{A} \in \mathcal{M}_{n\times m}(\mathbb{F})$, we have that $\boldsymbol{I}_n\boldsymbol{A} = \boldsymbol{A}\boldsymbol{I}_m = \boldsymbol{A}$.

2. Determinant and trace of square matrices

Let us now focus on the set $\mathcal{M}_{n\times n}(\mathbb{F})$ of square matrices and let us introduce two crucial scalar quantities that can be constructed using the entries of a square matrix.

DEFINITION 2.1 (*formal*). *Given a matrix $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{F})$, its determinant is given by*

$$\det \boldsymbol{A} = \sum_{\sigma\in S_n} \operatorname{sgn}(\sigma) \prod_{i=1}^{n} A_{i\,\sigma(i)}, \tag{3}$$

where the sum is taking over all permutations of elements $(1, 2, \ldots, n)$ and $\operatorname{sgn}(\sigma)$ is a sign or permutation.

This definition looks very abstract. For calculation purposes it is more convenient to use a different, but equivalent definition.

DEFINITION 2.2 (*inductive*). *The determinant of a square matrix $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{F})$ is provided by the so-called Laplace expansion alongs any row i*

$$\det \boldsymbol{A} = \sum_{j=1}^{n} (-1)^{i+j} A_{ij} \det \boldsymbol{A}^{(i,j)}. \tag{4}$$

Here the matrix $\boldsymbol{A}^{(i,j)}$ is the $(n-1)\times(n-1)$ matrix obtained removing the ith row and jth column from $\boldsymbol{A}$, and $\det \boldsymbol{A}^{(i,j)}$ is called the (i,j)-minor of $\boldsymbol{A}$.

If $\det \boldsymbol{A} = 0$ then $\boldsymbol{A}$ is *singular*. The reason for this nomenclature will be clear below.

THEOREM 2.1 (Properties of the determinant). *Let $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{F})$. Then*

- *if $\boldsymbol{A}$ is a diagonal matrix then $\det \boldsymbol{A} = \prod_{i=1}^{n} A_{ii}$.*
- *$\det \boldsymbol{A} = \det \boldsymbol{A}^{\top}$ (and therefore all properties referred to columns can be referred in terms of rows).*
- *For any constant $c \in \mathbb{F}$, $\det(c\boldsymbol{A}) = c^n \det \boldsymbol{A}$.*

- *Suppose that a column* $\boldsymbol{A}^k = \lambda \boldsymbol{v} + \boldsymbol{u}$*, i.e.,* $A_{ik} = \lambda U_k + V_k$*. Then*

$$\det \boldsymbol{A} = \det \begin{pmatrix} A_{11} & \dots & A_{1k} & \dots & A_{1n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{n1} & \cdots & A_{nk} & \cdots & A_{nn} \end{pmatrix}$$

$$= \lambda \det \begin{pmatrix} A_{11} & \dots & U_1 & \cdots & A_{1n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{n1} & \cdots & U_n & \cdots & A_{nn} \end{pmatrix} + \det \begin{pmatrix} A_{11} & \dots & V_k & \dots & A_{1n} \\ \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{n1} & \cdots & V_n & \cdots & A_{nn} \end{pmatrix}$$

  It is said that the determinant is multilinear.
- *If* $\det \boldsymbol{A}$ *has two identical columns, then* $\det \boldsymbol{A} = 0$*.*
- *Let* $\boldsymbol{B} \in \mathcal{M}_{n\times n}(\mathbb{F})$*, then* $\det \boldsymbol{AB} = \det \boldsymbol{A} \det \boldsymbol{B}$*.*

One of the consequences of the previous properties is that swapping two columns (or two rows) makes a minus sign appear in front of the determinant, i.e., the determinant is *alternating*,

$$\det \begin{pmatrix} A_{11} & \dots & A_{1k} & \dots & A_{1k'} & \dots & A_{1n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{n1} & \cdots & A_{nk} & \cdots & A_{nk'} & \cdots & A_{nn} \end{pmatrix}$$

$$= -\det \begin{pmatrix} A_{11} & \dots & A_{1k'} & \dots & A_{1k} & \dots & A_{1n} \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ A_{n1} & \cdots & A_{nk'} & \cdots & A_{nk} & \cdots & A_{nn} \end{pmatrix}$$

LEMMA 2.2. *Let* $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{F})$ *and* $\boldsymbol{C}$ *be its matrix of cofactors, i.e.,*

$$C_{ij} = (-1)^{i+j} \det \boldsymbol{A}^{(i,j)}.$$

Then if $\det \boldsymbol{A} \neq 0$*, the inverse of* $\boldsymbol{A}$ *exists and is given by*

$$\boldsymbol{A}^{-1} = \frac{1}{\det \boldsymbol{A}} \boldsymbol{C}^\top.$$

☞ It is possible to define a "pseudo–inverse matrix for non-square complex matrices (i.e., matrices with $\mathbb{F} = \mathbb{C}$). Such inverse is called *Moore-Penrose inverse* and is defined as follows. Suppose for simplicity that we work with complex numbers, $\mathbb{F} = \mathbb{C}$, and that $\boldsymbol{A} \in \mathcal{M}_{n\times m}(\mathbb{C})$. The matrix $\boldsymbol{A}^{-1}_{\mathrm{MP}} \in \mathcal{M}_{m\times n}(\mathbb{C})$ is the Moore-Penrose inverse of $\boldsymbol{A}$ if

(1) $\boldsymbol{A}\boldsymbol{A}^{-1}_{\mathrm{MP}}\boldsymbol{A} = \boldsymbol{A}$;
(2) $\boldsymbol{A}^{-1}_{\mathrm{MP}}\boldsymbol{A}\boldsymbol{A}^{-1}_{\mathrm{MP}} = \boldsymbol{A}^{-1}_{\mathrm{MP}}$;
(3) $\boldsymbol{A}\boldsymbol{A}^{-1}_{\mathrm{MP}}$ and $\boldsymbol{A}^{-1}_{\mathrm{MP}}\boldsymbol{A}$ are both Hermitian.

It can be shown that this pseudo inverse exists and is unique, and coincides with $\boldsymbol{A}^{-1}$ if $\boldsymbol{A}$ is square and non-singular.

As an example, consider the matrix $\boldsymbol{A} = (\frac{1}{2})$. Its Moore-Penrose inverse is equal to $\boldsymbol{A}^{-1}_{\mathrm{MP}} = (1/5, 2/5)$, which can be checked by direct calculations. It is easy to see that

$$\boldsymbol{A}\boldsymbol{A}^{-1}_{\mathrm{MP}} = \begin{pmatrix} 1/5 & 2/5 \\ 2/5 & 4/5 \end{pmatrix}, \qquad \boldsymbol{A}^{-1}_{\mathrm{MP}}\boldsymbol{A} = 1.$$

We conclude the section giving the following fundamental definition.

DEFINITION 2.3. *For a square matrix $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{F})$ we define its trace by*

$$\operatorname{tr} \boldsymbol{A} = \sum_{i=1}^{n} A_{ii}.$$

PROPOSITION 2.3. *Let be $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{C})$. Then*

$$\det \mathrm{e}^{\boldsymbol{A}} = \mathrm{e}^{\operatorname{tr} \boldsymbol{A}}.$$

3. Vector spaces

3.1. Definitions. Let us consider now the set of vectors $V \coloneqq \mathbb{F}^n \equiv \mathcal{M}_{n\times 1}(\mathbb{F})$ of column vectors. In this section, we will assume that $\mathbb{F} = \mathbb{R}$ or $\mathbb{F} = \mathbb{C}$. This set is a *vector space* over $\mathbb{F}$, i.e., is a set of elements such that, given $\boldsymbol{u}, \boldsymbol{v} \in \mathbb{F}^n$, then $\alpha\boldsymbol{v} + \beta\boldsymbol{u} \in \mathbb{F}$ for any $\alpha, \beta \in \mathbb{F}$. Given a set of K vectors $\{\boldsymbol{v}_k\}_{k=1,\dots,K}$, its *span* is the set

$$\operatorname{Span}[\{\boldsymbol{v}_k\}_k] = \left\{ \sum_{k=1}^{K} \alpha_k \boldsymbol{v}_k \colon \alpha_k \in \mathbb{F} \quad \forall k \right\}.$$

The set of K vectors $\{\boldsymbol{v}_k\}_{k=1}^{K}$ is said to be *linearly independent* if the equation $\sum_k \alpha_k \boldsymbol{v}_k = \boldsymbol{0}$ implies $\alpha_k = 0\ \forall k$. A *basis* is a set of linearly independent vectors which is *maximal*, i.e., such that adding any other set to the basis we obtain a set that is not linearly independent. This also means that if $\{\boldsymbol{e}_k\}_k$ is a basis of V, $V = \operatorname{Span}[\{\boldsymbol{e}_k\}_k]$. The cardinality of a basis of V is the *dimension* of V, and all basis have the same cardinality (if finite).

A vector space can be endowed with an *inner product* $\langle \bullet, \bullet \rangle \colon V \times V \to \mathbb{F}$, such that

$$\langle \boldsymbol{u}, \boldsymbol{v} \rangle = \sum_{i=1}^{n} \bar{u}_i v_i.$$

This inner product has many relevant properties.

- It is a *sesquilinear map*, $\langle \boldsymbol{u}, \alpha\boldsymbol{v}_1 + \beta\boldsymbol{v}_2 \rangle = \alpha\langle \boldsymbol{u}, \boldsymbol{v}_1 \rangle + \beta\langle \boldsymbol{u}, \boldsymbol{v}_2 \rangle$, but $\langle \alpha\boldsymbol{u}_1 + \beta\boldsymbol{u}_2, \boldsymbol{v} \rangle = \bar{\alpha}\langle \boldsymbol{u}_1, \boldsymbol{v} \rangle + \bar{\beta}\langle \boldsymbol{u}_2, \boldsymbol{v} \rangle$.
- It is antisymmetric, $\overline{\langle \boldsymbol{v}, \boldsymbol{u} \rangle} = \langle \boldsymbol{u}, \boldsymbol{v} \rangle$.

The set $\mathcal{M}_{n\times n}(\mathbb{F})$ is then a set of *linear maps* on V. Each $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{F})$ maps a vector $\boldsymbol{v} \in V$ into another vector $\boldsymbol{A}\boldsymbol{v} \in V$. The importance of linear maps motivated the study of their behavior when appearing inside inner products and led to the concept of *adjoint*. Given a matrix $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{F})$, we can define the *adjoint* of $\boldsymbol{A}$ as the matrix $\boldsymbol{A}^\dagger \in \mathcal{M}_{n\times n}(\mathbb{C})$ such that, in the notation above,

$$\langle \boldsymbol{u}, \boldsymbol{A}\boldsymbol{v} \rangle = \langle \boldsymbol{A}^\dagger \boldsymbol{u}, \boldsymbol{v} \rangle.$$

It is easy to see that to obtain $\boldsymbol{A}^\dagger$ from $\boldsymbol{A}$ you just need to transpose $\boldsymbol{A}$ and take the complex conjugate of all its elements: in other words, $\boldsymbol{A}^\dagger$ is the Hermitian transpose of $\boldsymbol{A}$, as the notation suggests.

3.1.1. *The bra-ket notation.* In many areas of modern physics people prefer to use the so called bra-ket notations to emphasize either we consider column or row vectors, so that the inner product $\langle \boldsymbol{u}, \boldsymbol{v} \rangle$ can be considered as a usual matrix product between a row vector obtained from $\boldsymbol{u}$ and the column vector $\boldsymbol{v}$.

DEFINITION 3.1. *Given a vector $\boldsymbol{u}$, we denote $\boldsymbol{u}^\dagger$ (i.e., the transpose complex conjugate) by the expression bra and write $\langle \boldsymbol{u}|$. We use instead the expression ket and write $|\boldsymbol{v}\rangle$ to denote a column vector $\boldsymbol{v} \in \mathcal{M}_{n\times 1}(\mathbb{C})$.*

In this way row vectors and column vectors are graphically distinguished. The product introduced above is rewritten as $\langle \boldsymbol{u}, \boldsymbol{v}\rangle = \langle \boldsymbol{u}|\boldsymbol{v}\rangle$. The duality operation † transforms a ket in a bra,

$$|\boldsymbol{a}\rangle \xrightarrow{\dagger} \langle \boldsymbol{a}|.$$

3.2. Rank of a matrix. We introduce now the concept of *rank*. First, let us consider the matrix $\boldsymbol{A} \in \mathcal{M}_{n\times m}(\mathbb{F})$, and let us call $\boldsymbol{a}^1, \ldots, \boldsymbol{a}^m$ the m columns of $\boldsymbol{A}$,

$$\boldsymbol{A} = \begin{pmatrix} \underbrace{A_{11}\\A_{21}\\A_{31}\\A_{41}}_{\boldsymbol{a}^1} & \underbrace{A_{12}\\A_{22}\\A_{32}\\A_{42}}_{\boldsymbol{a}^2} & \underbrace{A_{13}\\A_{23}\\A_{33}\\A_{43}}_{\boldsymbol{a}^3} \end{pmatrix} \tag{5}$$

Using the column vectors we define the following space.

Definition 3.2. *The linear span of the columns of a matrix is called column space.*

We can repeat the same argument with the *rows* of the matrix $\boldsymbol{A}$ and introduce the *row space* in the same way. Each one of these two spaces has a dimension, called *column rank* $r_c(\boldsymbol{A})$ for the column space and *row rank* $r_r(\boldsymbol{A})$ for the row space. The following fundamental results holds

Theorem 3.1. *For any matrix* $\boldsymbol{A}$, $r_c(\boldsymbol{A}) = r_r(\boldsymbol{A}) \equiv r(\boldsymbol{A})$. *The number* $r(\boldsymbol{A})$ *is called rank of* $\boldsymbol{A}$.

By definition, $r(\boldsymbol{A}) \leq \min\{n, m\}$. In the case of a square matrix $\boldsymbol{A}$ of size n, $\boldsymbol{A}$ is said to be *full rank* if $r(\boldsymbol{A}) = n$.

4. Spectral properties of square matrices

4.1. Eigenvalues and eigenvectors. In this section, we introduce a fundamental concept of invariance under the action of a square matrix $\boldsymbol{A}$. We will use the braket notation.

Definition 4.1. *Let* $|\boldsymbol{v}\rangle \in \mathcal{M}_{n\times 1}(\mathbb{C}) \equiv \mathbb{C}^n$ *be an* n*-dimensional vector and* $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{C})$ *be a square matrix. If the equation*

$$\boldsymbol{A}|\boldsymbol{v}\rangle = \lambda|\boldsymbol{v}\rangle$$

has a solution for some $\lambda \in \mathbb{C}$, *and* $|\boldsymbol{v}\rangle \neq |\boldsymbol{0}\rangle$, *then we say* λ *is an eigenvalue of* $\boldsymbol{A}$ *and* $|\mathbf{v}\rangle$ *is a right eigenvector of* $\boldsymbol{A}$. *Similarly, if we take a row vector* $\langle \boldsymbol{u}| \in \mathcal{M}_{1\times n}(\mathbb{C})$ *then*

$$\langle \boldsymbol{u}|\boldsymbol{A} = \lambda\langle \boldsymbol{u}|,$$

defines, for some $\lambda \in \mathbb{C}$, *and* $\langle \boldsymbol{u}| \neq \langle \boldsymbol{0}|$, *a left eigenvector.*

Observe that we distinguished between left and right eigenvalues but not between left and right eigenvalues. The reason is that left and right eigenvalues are actually the same, as we will see in a moment.

Each eigenvalue λ corresponds to infinitely many eigenvectors (as an example, if $\boldsymbol{v}$ is left eigenvector of $\boldsymbol{A}$ with eigenvalue λ, then $c\boldsymbol{v}$ is also left eigenvalue of $\boldsymbol{A}$ with the same eigenvalue). Each eigenvalue corresponds to an invariant *eigenspace*

whose dimension might be larger than 1. By definition, to find the set of eigenvalues (and eigenvectors) we have to solve

$$(\boldsymbol{A} - \lambda \boldsymbol{I}_n)\,|\boldsymbol{v}\rangle = |\boldsymbol{0}\rangle.$$

This equation has a nontrivial solution if, and only if

$$p_{\boldsymbol{A}}(\lambda) \coloneqq \det(\boldsymbol{A} - \lambda \boldsymbol{I}_n) = 0$$

(otherwise $\boldsymbol{A} - \lambda \boldsymbol{I}_n$ would be invertible and we would find $\boldsymbol{v} = \boldsymbol{0}$). The determinant is a polynomial in λ of degree n, which is known as *characteristic polynomial*. In general the polynomial $p_{\boldsymbol{A}}(\lambda)$ has n roots (some of them possibly identical) in $\mathbb{C}$. We could repeat the same arguments using the equation for the left eigenvectors: we would have found the *same* characteristic polynomial: this implies, as anticipated, that left and right eigenvalues are the same. The following important proposition holds.

PROPOSITION 4.1. *Hermitian matrices have only real eigenvalues. Moreover, if $|\boldsymbol{v}\rangle$ is a left eigenvector of an Hermitian matrix $\boldsymbol{A}$, then $\langle \boldsymbol{v}|$ is a right eigenvector of the same matrix, and vice versa.*

Moreover, let $|\boldsymbol{u}\rangle$ and $|\boldsymbol{v}\rangle$ be two right eigenvectors of a Hermitian matrix $\boldsymbol{A}$ corresponding to eigenvalues λ and μ respectively, with $\lambda \neq \mu$. Then $\langle \boldsymbol{u}|\boldsymbol{v}\rangle = 0$, i.e., they are orthogonal.

There is one subclass of Hermitian matrices which is widely used in many applications.

DEFINITION 4.2. *An Hermitian matrix $\boldsymbol{A}$ of size n is called positive definite if for any vector $|\boldsymbol{v}\rangle \neq |\boldsymbol{0}\rangle$ we have $\langle \boldsymbol{v}|\boldsymbol{A}|\boldsymbol{v}\rangle > 0$.*

PROPOSITION 4.2. *All eigenvalues of positive definite matrix are positive.*

Finally, let us state an important theorem on square matrices with real entries.

THEOREM 4.3 (O. Perron, F.G. Frobenius). *Let $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{R})$ such that $A_{ij} \geq 0\ \forall i, j \in \{1, \dots, n\}$. Then there is an eigenvalue of $\boldsymbol{A}$ such that $\lambda_{\mathrm{PF}} \in \mathbb{R}$, $\lambda_{\mathrm{PF}} \geq 0$ and the associated (left and right) eigenvectors have non-negative entries. Moreover, for any other eigenvalue λ one has $|\lambda| \leq \lambda_{\mathrm{PF}}$.*

4.2. Spectral decomposition. There are many ways to decompose a matrix and the choice usually depends on the problem that has to be solved. Here we will discuss perhaps the most fundamental, the *spectral decomposition*.

THEOREM 4.4 (Matrix spectral decomposition). *Let $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{C})$ and suppose that there are n linearly independent right eigenvectors, $|\boldsymbol{v}_1\rangle, \dots, |\boldsymbol{v}_n\rangle$. Then $\boldsymbol{A}$ can be factorized as*

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{-1}$$

where $\boldsymbol{\Lambda} = \operatorname{diag}(\lambda_1, \dots, \lambda_n)$ is a diagonal matrix having $\Lambda_{ij} = \lambda_i \delta_{ij}$ and $\boldsymbol{Q}$ is the matrix whose j-th column is equal to $|\boldsymbol{v}_j\rangle$.

Not any matrix can be decomposed into such a product: indeed, the condition of having *n linearly independent eigenvectors* is essential, and this is not true for any square matrix on $\mathbb{C}$. If $\boldsymbol{A}$ has the spectral decomposition described above, then any integer power of $\boldsymbol{A}$ can be easily calculated as

$$\boldsymbol{A}^k = \boldsymbol{Q}\boldsymbol{\Lambda}^k\boldsymbol{Q}^{-1}.$$

The spectral decomposition recasts a matrix in terms of its eigenvalues and eigenvectors. This representation turns out to be enormously useful. We additionally specify the properties of the eigenvectors in the case of Hermitian matrices.

THEOREM 4.5 (Spectral decomposition for real-symmetric matrices). *Let $\boldsymbol{A}$ be any real symmetric matrix of size n with eigenvalues $\lambda_1, \ldots, \lambda_n$ and corresponding orthonormal eigenvectors $|\boldsymbol{v}_1\rangle, \ldots, |\boldsymbol{v}_n\rangle$. Let $\boldsymbol{Q}$ be a matrix with columns $|\boldsymbol{v}_1\rangle, \ldots, |\boldsymbol{v}_n\rangle$. Then, in the notation above,*

$$\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^\top = \sum_{k=1}^{n} \lambda_k |\boldsymbol{v}_k\rangle\langle\boldsymbol{v}_k|.$$

The matrix $\boldsymbol{Q}$ is orthogonal, i.e. $\boldsymbol{Q}\boldsymbol{Q}^\top = \boldsymbol{Q}^\top\boldsymbol{Q} = \boldsymbol{I}_n$.

THEOREM 4.6 (Spectral decomposition for Hermitian matrices). *Let $\boldsymbol{A}$ be any Hermitian matrix of size n with eigenvalues $\lambda_1, \ldots, \lambda_n$ and corresponding orthonormal eigenvectors $|\boldsymbol{v}_1\rangle, \ldots, |\boldsymbol{v}_n\rangle$. Let $\boldsymbol{U}$ be a matrix with columns $|\boldsymbol{v}_1\rangle, \ldots, |\boldsymbol{v}_n\rangle$. Then*

$$\boldsymbol{A} = \boldsymbol{U}\boldsymbol{\Lambda}\boldsymbol{U}^\dagger = \sum_{k=1}^{n} \lambda_k |\boldsymbol{v}_k\rangle\langle\boldsymbol{v}_k|.$$

The matrix $\boldsymbol{U}$ is unitary, i.e. $\boldsymbol{U}\boldsymbol{U}^\dagger = \boldsymbol{U}^\dagger\boldsymbol{U} = \boldsymbol{I}_n$. In the special case in which $\boldsymbol{A}$ is real symmetric, then the orthonormal eigenvectors are vectors of real quantities and the matrix $\boldsymbol{U}$ is an orthogonal matrix.

4.3. Functions over $\mathcal{M}_{n\times n}(\mathbb{C})$. Assume that we have some analytic function $f\colon \mathbb{C} \to \mathbb{C}$. How could we define $f(\boldsymbol{A})$ for $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{C})$? This is an easy question if f is a polynomial, but less obvious if it is, e.g., an exponential. However, if $\boldsymbol{A}$ is diagonalizable as $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{-1}$, then for any integer power k we have $\boldsymbol{A}^k = \boldsymbol{Q}\boldsymbol{\Lambda}^k\boldsymbol{Q}^{-1}$. Now let us use Taylor expansion of function $f(x)$ around zero. Assuming that f is analytic in a neighbourhood of the origin, we can write

$$f(z) = \sum_{k=0}^{\infty} a_k z^k.$$

It is natural to define $f(\boldsymbol{A})$ as

$$f(\boldsymbol{A}) = \sum_{k=0}^{\infty} a_k \boldsymbol{Q}\boldsymbol{\Lambda}^k\boldsymbol{Q}^{-1} = \boldsymbol{Q}\, f(\boldsymbol{\Lambda})\, \boldsymbol{Q}^{-1}.$$

$\boldsymbol{\Lambda}$ is a diagonal matrix with $\Lambda_{ij} = \lambda_i\delta_{ij}$, so that $[\boldsymbol{\Lambda}^k]_{ij} = \lambda_i^k\delta_{ij}$. As a result,

$$f(\boldsymbol{\Lambda}) = \operatorname{diag}\left(f(\lambda_1), \ldots, f(\lambda_n)\right)$$

so that we can give the following definition

DEFINITION 4.3. *Let $f\colon \mathbb{C} \to \mathbb{C}$ be an analytic function around the origin. Then for any diagonalizable matrix $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{-1}$ we define*

$$f(\boldsymbol{A}) \coloneqq \boldsymbol{Q}\, \operatorname{diag}\left(f(\lambda_1), \ldots, f(\lambda_n)\right)\, \boldsymbol{Q}^{-1}.$$

EXAMPLE Let us calculate $\exp(\boldsymbol{A})$ with

$$\boldsymbol{A} = \begin{pmatrix} 1 & 0 \\ -4/3 & 2 \end{pmatrix}.$$

First we need to find eigenvalues and corresponding eigenvectors. To find the eigenvalues, we write $\det(\boldsymbol{A} - \lambda \boldsymbol{I}_2) = 0$ to get $\lambda_1 = 1$ and $\lambda_2 = 2$. The right eigenvalues can be found as $|\boldsymbol{v}_1\rangle = \binom{3}{4}$ and $|\boldsymbol{v}_1\rangle = \binom{0}{1}$. Then taking

$$\boldsymbol{Q} = \begin{pmatrix} 3 & 0 \\ 4 & 1 \end{pmatrix}, \quad \boldsymbol{\Lambda} = \begin{pmatrix} 1 & 0 \\ 0 & 2 \end{pmatrix},$$

we obtain $\boldsymbol{A} = \boldsymbol{Q}\boldsymbol{\Lambda}\boldsymbol{Q}^{-1}$. Therefore,

$$\exp(\boldsymbol{A}) = \boldsymbol{Q}\mathrm{diag}\left(\mathrm{e}, \mathrm{e}^2\right)\boldsymbol{Q}^{-1} = \begin{pmatrix} \mathrm{e} & 0 \\ \frac{4}{3}\left(\mathrm{e} - \mathrm{e}^2\right) & \mathrm{e}^2 \end{pmatrix}.$$

EXAMPLE For non-diagonalizable functions there is no general recipe, however sometimes it is still possible to calculate corresponding values. Let us take

$$\boldsymbol{A} = \begin{pmatrix} 1 & 1 \\ 0 & 1 \end{pmatrix},$$

and $f(z) = \mathrm{e}^z$. We will try to approach this problem by using Taylor series expansion. But we need to find a way of calculating integer powers of matrix $\boldsymbol{A}$. Several first powers are easy to get and equal to

$$\boldsymbol{A}^2 = \begin{pmatrix} 1 & 2 \\ 0 & 1 \end{pmatrix}, \quad \boldsymbol{A}^3 = \begin{pmatrix} 1 & 3 \\ 0 & 1 \end{pmatrix}, \quad \boldsymbol{A}^4 = \begin{pmatrix} 1 & 4 \\ 0 & 1 \end{pmatrix}, \qquad \text{etc.}$$

One can now guess (and proof by induction) that

$$\boldsymbol{A}^k = \begin{pmatrix} 1 & k \\ 0 & 1 \end{pmatrix}.$$

Therefore,

$$\exp(\boldsymbol{A}) = \sum_{k=0}^{\infty} \frac{1}{k!} \begin{pmatrix} 1 & k \\ 0 & 1 \end{pmatrix} = \mathrm{e}\,\boldsymbol{A}.$$

Exercises

(1) Calculate the determinant of the following *Vandermonde matrix*

$$\begin{pmatrix} 1 & x_1 & x_1^2 & x_1^3 \\ 1 & x_2 & x_2^2 & x_2^3 \\ 1 & x_3 & x_3^2 & x_3^3 \\ 1 & x_4 & x_4^2 & x_4^3. \end{pmatrix}$$

Try to generalize the last determinant to the case of any matrix size.

(2) Prove Proposition 2.3 for any real symmetric (or Hermitian) matrix $\boldsymbol{A}$. *Hint:* use the definition of matrix exponent via its spectral decomposition.

LECTURE 2

Calculus

1. Infinite series, power series and Taylor series expansion

DEFINITION 1.1. *Given an infinite ordered sequence of number*

$$(a_n)_n = (a_1, \dots, a_k, \dots), \qquad a_k \in \mathbb{F} \text{ for all } k,$$

the corresponding infinite series is an expression of the form

$$a_1 + \cdots + a_k + \ldots \coloneqq \sum_{k=1}^{\infty} a_k.$$

The elements of the sequence can belong to a set that is not a field: it is indeed enough to have the structure of abelian group. This is for example the case of $\mathcal{M}_{n\times m}(\mathbb{F})$ with the operation of matrix addition. In the following, we will focus on sequence of *real numbers*, i.e., $\mathbb{F} = \mathbb{R}$. The case $\mathbb{F} = \mathbb{C}$ is easily obtained observing that a series of complex number can be obtained considering separately a series of their real and imaginary part. Similarly, a series of matrices $\mathcal{M}_{n\times m}(\mathbb{C})$ can be reduced to a series of reals looking at the sums component-wise.

It is easy to think to series corresponding to values of the sum that is not a finite quantity, for example $\sum_{k\in\mathbb{N}} k$. On the other hand, we would like to give a more precise definition of what is the "sum" of the series when it converges (somehow) to a finite number. This can be formally defined defined by using the following

DEFINITION 1.2. *A partial sum of an infinite series $S = \sum_{k=1}^{\infty} a_k$ is the quantity*

$$S_n = \sum_{k=1}^{n} a_k$$

for any $n \geq 1$. The series $S = \sum_{k=1}^{\infty} a_k$ is said to be convergent if

$$S = \lim_{n\to\infty} S_n$$

exists finite. This limit is called the sum of series. The series is otherwise said to be divergent.

EXAMPLE For a series $S = \sum_{k=1}^{\infty} a^{-k}$ with $a > 1$ we have $S_n = \frac{1-a^{-n}}{a-1}$ so that $S = \lim_{n\to+\infty} S_n = \frac{1}{a-1}$.

EXAMPLE For a series $S = \sum_{k=1}^{\infty} k$ we have $S_n = \frac{n(n+1)}{2} \xrightarrow{n\to+\infty} +\infty$ and the series diverges.

One of the main consequences of the above definition is that there is an important, necessary condition for a series to be convergent. Indeed, if $S_n \to S$, then $S_n - S_{n-1} = a_n \to 0$ for $n \to +\infty$ This is however not a sufficient condition, a classical example being the harmonic series.

EXAMPLE: THE HARMONIC SERIES The harmonic series is

$$\sum_{k=1}^{\infty} \frac{1}{k}.$$

In this series $a_n \to 0$ but the series is divergent. Indeed,

$$S_{2n} - S_n = \sum_{k=n+1}^{2n} \frac{1}{k} > \sum_{n=n+1}^{2n} \frac{1}{2n} = \frac{1}{2},$$

which means that the sequence S_N does not converge to a limit.

Below we state several tests which can be used to determine whether a real series is convergent or divergent.

THEOREM 1.1 (The limit comparison test). *If both $a_k, b_k \geq 0$ and if $\lim_{k\to\infty} \frac{a_k}{b_k}$ exists, then either both series $\sum_{k=1}^{\infty} a_k$ and $\sum_{k=1}^{\infty} b_k$ are convergent or both series are divergent.*

THEOREM 1.2 (The n-th root test). *For a series $S = \sum_{k=1}^{\infty} a_k$, if*

$$\limsup_{k\to\infty} \sqrt[k]{|a_k|} < 1$$

then the series converges. On the other hand, if

$$\limsup_{k\to\infty} \sqrt[k]{|a_k|} > 1$$

the series diverges.

THEOREM 1.3 (The ratio test). *For a series $S = \sum_{k=1}^{\infty} a_k$, if*

$$\limsup_{k\to\infty} \left| \frac{a_{k+1}}{a_k} \right| < 1$$

then the series converges. On the other hand, if

$$\limsup_{k\to\infty} \left| \frac{a_{k+1}}{a_k} \right| > 1$$

the series diverges.

In both Theorems 1.2 and 1.3 one can change $\limsup_k b_k$ to the proper limit $\lim_k b_k$ as long as it exists. We draw attention to the fact that in Theorems 1.2 and 1.3 certain cases are omitted, and, specifically when the limits are equal to one, the root and the ratio tests are both inconclusive.

EXAMPLE Let us consider series $S = \sum_{k=1}^{\infty} \sin kx$ for $x \in \mathbb{R}$. The k-th term of the series is equal to $\sin kx$ and obviously doesn't converge to 0 if x is not a multiple of π. But if $x = k\pi$ for some $k \in \mathbb{Z}$, then all terms in the series are zeros and the series converges.

EXAMPLE The series $S = \sum_{k=1}^{\infty} \frac{k^2}{\left(2+\frac{1}{k}\right)^k}$ converges. This can be seen using the root test. Indeed,

$$\sqrt[k]{a_k} = \frac{\left(\sqrt[k]{k}\right)^2}{2+\frac{1}{k}} \to \frac{1}{2},$$

which means that the series is convergent.

1.1. Power series. Let us now focus on a special type of series, of great relevance for applications.

DEFINITION 1.3. *A power series is a formal expression of the form*

$$S(x) = \sum_{k=k_0}^{\infty} c_k (x-\alpha)^k$$

for some $\alpha \in \mathbb{R}$ and some $k_0 \in \mathbb{Z}$.

If we fix x, a power series is a usual series of the type $\sum_{k \geq k_0} a_k$ with $a_k = c_k(x-\alpha)^k$ and, in this sense, to $S(x)$ as family of series whose elements are labeled by x. The n-th root test tells us that that the power series is convergent if

$$|x-\alpha| < \left(\limsup_{k\to\infty} \sqrt[k]{|c_k|} \right)^{-1}$$

and diverges if

$$|x-\alpha| > \left(\limsup_{k\to\infty} \sqrt[k]{|c_k|} \right)^{-1}.$$

This means that there is a *radius of convergence* of the series.

DEFINITION 1.4. *The radius of convergence of a power series $S(x) = \sum_{k=k_0}^{\infty} c_k(x-\alpha)^k$ is a non-negative number R such that the series converges for $|x-\alpha| < R$, where*

$$R = \left(\limsup_{k\to\infty} \sqrt[k]{|c_k|} \right)^{-1}. \tag{6}$$

The radius can be computed also using

$$R = \left(\limsup_{k\to\infty} \left| \frac{c_{k+1}}{c_k} \right| \right)^{-1} \tag{7}$$

when this limit exists. The open ball $|x-\alpha| < R$ is called ball of convergence $\mathcal{B}(\alpha, R)$.

Note that on the boundary $|x-\alpha| < R$ we cannot give any information by this method. If $R = 0$ then the series diverges for all $x \neq \alpha$. On the other hand, if $R = \infty$ then the series converges for all $x \in \mathbb{R}$. Finally, we remark here that the limit $R = \left(\limsup_{k\to\infty} \left| \frac{c_{k+1}}{c_k} \right| \right)^{-1}$ is often simpler to compute, but it only exists if the power series has nonzero consecutive terms.

EXAMPLE Let us find radius and ball of convergence for

$$S(x) = \sum_{n=1}^{\infty} \frac{3^{2n} n!^3}{(3n)!} (x-1)^n .$$

Using (7) we obtain

$$R = \left(\limsup_{n\to\infty} \left| \frac{9\,(n+1)^3}{(3n+1)\,(3n+2)\,(3n+3)} \right| \right)^{-1} = 3.$$

Therefore, series is convergent for $x \in (-2, 4)$.

A convergent power series defines a function $S(x)$ inside its ball of convergence. Let us assume from now on that $k_0 = 0$. Proceeding in a heuristic way, we can observe that

$$\frac{\mathrm{d}\, S(x)}{\mathrm{d}\, x} = \sum_{k=1}^{\infty} c_k k (x-\alpha)^{k-1}$$

and more generally

$$\frac{\mathrm{d}^n\, S(x)}{\mathrm{d}\, x^n} = \sum_{k=n}^{\infty} \frac{c_k k!}{(k-n)!} (x-\alpha)^{k-n}$$

This implies that

$$S^{(n)}(\alpha) \coloneqq \left. \frac{\mathrm{d}^n\, S(x)}{\mathrm{d}\, x^n} \right|_{x=\alpha} = c_n n! \Longrightarrow c_n = \frac{1}{n!} \left. \frac{\mathrm{d}^n\, S(x)}{\mathrm{d}\, x^n} \right|_{x=\alpha} .$$

We may wonder if, given a function f, we can use this recipe to perform the opposite operation, i.e., construct a series converging to f in some part of its domain given f. The answer is *yes* and such a series can be constructed using a *Taylor expansion.*

DEFINITION 1.5. *The Taylor series around the point $x = \alpha$ of an infinitely differentiable function $f(x) \in C^\infty(\mathcal{B}(\alpha, R))$ is given by*

$$f(x) = \sum_{k=0}^{\infty} \frac{f^{(k)}(\alpha)}{k!} (x-\alpha)^k .$$

EXAMPLE Let us consider function $f(x) = \mathrm{e}^x$ and find its Taylor series expansion in around point $x = 0$. For any $k \geq 0$ we have $f^{(k)}(x) = \mathrm{e}^x$. Therefore,

$$f(x) = \sum_{n=0}^{\infty} \frac{x^n}{n!}.$$

EXAMPLE Sometimes it is easier to find Taylor series expansion of a part of the function and then work out the whole series. For example let us take $f(x) = \frac{\mathrm{e}^x - x - 1}{x^2}$ around $x = 0$. Instead of working with the entire entire expression, if we take Taylor series of the numerator

$$\mathrm{e}^x - x - 1 = \sum_{k=0}^{\infty} \frac{x^k}{k!} - x - 1 = \sum_{k=2}^{\infty} \frac{x^k}{k!} = \sum_{k=0}^{\infty} \frac{x^{k+2}}{(k+2)!}$$

and then divide it by x^2, we will easily get an answer

$$f(x) = \sum_{k=0}^{\infty} \frac{x^k}{(k+2)!}.$$

One of the main applications of the Taylor series expansion is the approximation of a given function f by a polynomial in some region of the domain of f. The following theorem provides a measure of the quality of this approximation.

THEOREM 1.4 (Taylor). *Let $f(x) \in C^{n+1}(\mathcal{B}(\alpha, R))$. Then for any $x \in \mathcal{B}(\alpha, R)$*

$$f(x) = \sum_{k=0}^{n} \frac{f^{(k)}(\alpha)}{k!} (x-\alpha)^k + R_{n+1}(x),$$

where the remainder is such that

$$R_{n+1}(x) = \frac{f^{(n+1)}(X)}{(n+1)!}(x-\alpha)^{n+1},$$

for some $X \in \mathcal{B}(\alpha, R)$. This means that

$$|R_{n+1}(x)| \leq \frac{\max_{X \in \mathcal{B}(\alpha,R)} \left|f^{(n+1)}(X)\right|}{(n+1)!} |x-\alpha|^{n+1}.$$

EXAMPLE Let us find value of e^z, $z > 0$, with an error not more than $\varepsilon = 0.01$. We will use Taylor series expansion of $f(x) = \mathrm{e}^x$ in around 0. This means that we want the reminder to be less then ϵ focusing on the ball $\mathcal{B}(0, z)$. In other words, we want n such that

$$\frac{\max_{X \in \mathcal{B}(0,z)} \mathrm{e}^X z^{n+1}}{(n+1)!} = \frac{\mathrm{e}^z z^{n+1}}{(n+1)!} < \varepsilon$$

For example, for $z = 0.2$ this is satisfied for $n = 2$. Indeed in this case

$$1 + 0.2 + \frac{(0.2)^2}{2} = 1.22$$

to be compared with the exact value $1.2214027581601698339210\ldots$

We conclude this brief paragraph on power series with the following

DEFINITION 1.6. *A function which can be locally written as a convergent power series in its entire domain is called an analytic function.*

This means that f is anaylitic if for any α in the domain of f, it can be written as a Taylor series within $\mathcal{B}(\alpha, R)$ for a nonzero R convergent for some non-zero radius R. In this case, as we can always find a convergent power series expansion, then the function f is continuous and differentiable in all points of its domain.

2. Some tools for integration

2.1. Changing variables in multidimensional integrals. In this section we recall how to perform a change of variable when preforming multivariate integrals. Given a function $\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^n$, in the following we will use the notation

$$\partial_\nu f^\mu(\boldsymbol{x}) \coloneqq \frac{\partial f^\mu(\boldsymbol{x})}{\partial x_\nu}.$$

Let us first introduce

DEFINITION 2.1 (Jacobian). *Let $\boldsymbol{f} : \mathbb{R}^m \to \mathbb{R}^n$ be a vector valued function. Matrix $\boldsymbol{J_f}$ of all first order partial derivatives of function f is called Jacobian matrix, i.e.*

$$\boldsymbol{J_f}(\boldsymbol{x}) = \begin{pmatrix} \partial_1 f^1(\boldsymbol{x}) & \partial_2 f^1(\boldsymbol{x}) & \dots & \partial_m f^1(\boldsymbol{x}) \\ \partial_1 f^2(\boldsymbol{x}) & \partial_2 f^2(\boldsymbol{x}) & \dots & \partial_m f^1(\boldsymbol{x}) \\ \vdots & \vdots & \ddots & \vdots \\ \partial_1 f^n(\boldsymbol{x}) & \partial_2 f^n(\boldsymbol{x}) & \dots & \partial_m f^n(\boldsymbol{x}) \end{pmatrix}.$$

If $n = m$, the determinant of the Jacobian matrix is simply called Jacobian.

The following theorem provides a recipe to perform a change of variable in multivariate integrals.

THEOREM 2.1. *Let D be an open set in $\mathbb{R}^n$ and $\boldsymbol{\phi} : D \to \mathbb{R}^n$ an injective differentiable function with continuous partial derivatives, the Jacobian of which is non-zero for every $\boldsymbol{x} \in D$. Then for any real-valued, compactly supported, continuous function f, with support contained in $\boldsymbol{\phi}(D)$, we have*

$$\int\limits_{\boldsymbol{\phi}(D)} f(\boldsymbol{x}) \,\mathrm{d}\,\boldsymbol{x} = \int\limits_{D} f\left(\boldsymbol{\phi}(\boldsymbol{y})\right) \left|\det \boldsymbol{J}_{\boldsymbol{\phi}}(\boldsymbol{y})\right| \mathrm{d}\,\boldsymbol{y},$$

where $\boldsymbol{J}_{\boldsymbol{\phi}}$ is the Jacobian of function $\boldsymbol{\phi}$ and $\mathrm{d}\,\boldsymbol{x} = \prod_{j=1}^{n} \mathrm{d}\,x_j$, $\mathrm{d}\,\boldsymbol{y} = \prod_{j=1}^{n} \mathrm{d}\,y_j$.

COROLLARY 2.2. *Let $D = \mathbb{R}^n$ and $\boldsymbol{A} \in \mathcal{M}_{n\times n}(\mathbb{R})$, so that we want to perform the change of variable $\boldsymbol{\phi}\colon \boldsymbol{x} \mapsto \boldsymbol{A}\boldsymbol{x}$. Then $\boldsymbol{J}_{\boldsymbol{\phi}} = \boldsymbol{A}$ and corresponding change of variables formula will take the form*

$$\int\limits_{\mathbb{R}^n} f(\boldsymbol{x}) \,\mathrm{d}\,\boldsymbol{x} = \left|\det \boldsymbol{A}\right| \int\limits_{\mathbb{R}^n} f\left(\boldsymbol{A}\boldsymbol{y}\right) \mathrm{d}\,\boldsymbol{y}.$$

EXAMPLE: POLAR COORDINATES CHANGE Let us calculate the area of the domain

$$D = \{(x, y) \in \mathbb{R}^2 \colon x^2 + y^2 \geq 1 \text{ and } \left(x^2 + y^2\right)^2 \leq 2\left(x^2 - y^2\right)$$

By the definition of area, we have

$$\operatorname{area}(D) = \int\limits_{D} \mathrm{d}\,x \,\mathrm{d}\,y.$$

In the above integral, we perform a change of variables to polar ones

$$\boldsymbol{\phi}\colon \begin{pmatrix} x \\ y \end{pmatrix} \mapsto \begin{pmatrix} r\cos\varphi \\ r\sin\varphi \end{pmatrix}$$

with $r \in \mathbb{R}_+$ and $\varphi \in [-\pi, \pi)$. In this new set of variables the domain is written as

$$D = \{(r\cos\varphi, r\sin\varphi) \in \mathbb{R}^2 \colon r^2 \geq 1 \text{ and } r^2 \leq 2\cos 2\varphi \text{ and } \varphi \in [-\pi, \pi]\}$$

Combining all the above we get

$$\operatorname{area}(D) = 2\int\limits_{-\pi}^{\pi} \theta(\cos 2\varphi) \,\mathrm{d}\,\varphi \int\limits_{1}^{\sqrt{2\cos 2\varphi}} \mathrm{d}\,r \left|\det \boldsymbol{J}_{\boldsymbol{\phi}}(r, \varphi)\right|.$$

Calculating the Jacobian we get

$$\det \boldsymbol{J}_{\boldsymbol{\phi}}(r, \varphi) = \begin{vmatrix} \partial_r x & \partial_r y \\ \partial_\varphi x & \partial_\varphi y \end{vmatrix} = \begin{vmatrix} \cos\varphi & \sin\varphi \\ -r\sin\varphi & r\cos\varphi \end{vmatrix} = r.$$

And finally

$$\operatorname{area}(D) = 2\int\limits_{-\pi/6}^{\pi/6} \mathrm{d}\,\varphi \int\limits_{1}^{\sqrt{2\cos 2\varphi}} r\,\mathrm{d}\,r = \int\limits_{-\pi/6}^{\pi/6} (2\cos 2\varphi - 1)\,\mathrm{d}\,\varphi = \sqrt{3} - \frac{\pi}{3}.$$

2.2. Single and multi variable Gaussian integrals. In this section we discuss several examples of the integrals containing exponents of quadratic forms in $\mathbb{R}^n$, i.e., expressions of the type

$$L(\boldsymbol{x}) = \langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle,$$

where $\boldsymbol{A}$ is a *real symmetric matrix* in $\mathcal{M}_{n\times n}(\mathbb{R})$. Observe that the assumption of having $\boldsymbol{A}$ real symmetric is not restrictive: one can also easily get that for any non symmetric matrix $\boldsymbol{A}$ $\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle = \left\langle \boldsymbol{x}, \frac{\boldsymbol{A}+\boldsymbol{A}^\top}{2}\boldsymbol{x}\right\rangle$, where obviously $\frac{\boldsymbol{A}+\boldsymbol{A}^\top}{2}$ is now symmetric.

Definition 2.2. *For any quadratic form in $\mathbb{R}^n$ with associated real positive symmetric matrix $\boldsymbol{A}$ and function $f : \mathbb{R}^n \to \mathbb{R}$ we define Gaussian integral of general form by*

$$I\,(f;\boldsymbol{A}) = \int\limits_{\mathbb{R}^n} f(\boldsymbol{x})\,\mathrm{e}^{-\frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle}\,\mathrm{d}\,\boldsymbol{x}.$$

Below we state some well-known results on Gaussian integrals without proofs.

- If $f(\boldsymbol{x}) \equiv 1$ for all $\boldsymbol{x} \in \mathbb{R}^n$,

$$\int\limits_{\mathbb{R}^n} \mathrm{e}^{-\frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle}\,\mathrm{d}\,\boldsymbol{x} = \frac{(2\pi)^{\frac{n}{2}}}{\sqrt{\det \boldsymbol{A}}} \text{ and in particular } \int\limits_{\mathbb{R}} \mathrm{e}^{-\frac{1}{2}Ax^2}\,\mathrm{d}\,x = \sqrt{\frac{2\pi}{A}}. \tag{8}$$

- If $f(\boldsymbol{x}) = \mathrm{e}^{\langle \boldsymbol{b}, \boldsymbol{x}\rangle}$ for some n-dimensional vector $\boldsymbol{b}$, then

$$\int\limits_{\mathbb{R}^n} \mathrm{e}^{\langle \boldsymbol{b}, \boldsymbol{x}\rangle - \frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle}\,d\boldsymbol{x} = \frac{(2\pi)^{\frac{n}{2}}\,\mathrm{e}^{\left\langle \boldsymbol{b}, \boldsymbol{A}^{-1}\boldsymbol{b}\right\rangle}}{\sqrt{\det \boldsymbol{A}}}, \tag{9}$$

$$\text{in particular } \int\limits_{\mathbb{R}} \mathrm{e}^{bx - \frac{Ax^2}{2}}\,\mathrm{d}\,x = \sqrt{\frac{2\pi}{A}}\,\mathrm{e}^{\frac{b^2}{2A}}.$$

- $f(\boldsymbol{x})$ is a product of even number of coordinates

$$\int\limits_{\mathbb{R}^n} x_j x_k\,\mathrm{e}^{-\frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle}\,\mathrm{d}\,\boldsymbol{x} = \frac{(2\pi)^{\frac{n}{2}}\,[\boldsymbol{A}^{-1}]_{j,k}}{\sqrt{\det \boldsymbol{A}}}, \text{ in particular } \int\limits_{\mathbb{R}} x^2\,\mathrm{e}^{-\frac{Ax^2}{2}}\,\mathrm{d}\,x = \sqrt{\frac{2\pi}{A^3}}.$$

$$\int\limits_{\mathbb{R}^n} \prod_{j=1}^{2m} x_{k_j}\,\mathrm{e}^{-\frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle}\,\mathrm{d}\,\boldsymbol{x} = \frac{(2\pi)^{\frac{n}{2}}}{\sqrt{\det \boldsymbol{A}}}\frac{1}{2^m m!}\sum_{\sigma\in S_{2m}}\prod_{j=1}^{m}[\boldsymbol{A}^{-1}]_{k_{\sigma(2j-1)},k_{\sigma(2j)}}.$$

2.3. Gaussian linearisation or Hubbard-Stratonovich trick. The so-called Hubbard-Stratonovich transformation in dimension $n = 1$ is simply a simple one-dimensional Gaussian integral involving complex quantities. The main advantage of the formula is the fact that transforms an exponent of quadratic form in x into another exponent which is linear in x by introducing new auxiliary variables.

PROPOSITION 2.3 (Hubbard-Stratonovich transformation). *For any $x, A \in \mathbb{C}$ such that $\Re A > 0$*

$$\exp\left\{-\frac{Ax^2}{2}\right\} = \frac{1}{\sqrt{2\pi A}} \int_{-\infty}^{\infty} \exp\left\{-\frac{y^2}{2A} + ixy\right\} \mathrm{d}\, y.$$

The interesting aspect of this identity is that can be generalised to various cases in which, for example, x is a complex object such as an operator. Sometimes the Hubbard-Stratonovich formula is also used to reduce exponential of x^4 to exponential of x^2.

3. Asymptotic analysis

Asymptotic approximation is an important topic in applied analysis, and its applications permeate many fields in science and engineering such as fluid mechanics, electromagnetism, diffraction theory, and statistics. In analysis and applied mathematics, one frequently comes across problems concerning the determination of the behaviour of a function as one of its parameters tends to a specific value, or of a sequence as its index tends to infinity. Thus, for instance, results such as

$$\log n! \sim \left(n + \frac{1}{2}\right) \log n - n + \frac{1}{2} \log 2\pi,$$

called Stirling's approximation. The twiddle sign $\sim$ is used to mean that the quotient of the left-hand side by the corresponding right-hand side approaches 1 as $n \to \infty$. The present subject of asymptotics deals with functions that are expressible in the forms of definite integrals or contour integrals. A typical example in this area is given by the integral

$$I_n = \int_a^b \phi(x) \left(\psi(x)\right)^n \mathrm{d}\, x,$$

where $\phi(x)$ and $\psi(x)$ are continuous functions defined on the interval $[a, b]$ and $\psi(x)$ is positive there. The main subject of the following is to build an asymptotic expansion for such integrals. First we define an asymptotic scale, and then give the formal definition of an asymptotic expansion.

DEFINITION 3.1. *If $\{\phi_n(z)\}_{n=0}^{\infty}$ is a sequence of continuous functions on some domain $\Omega \subset \mathbb{C}$, and if z_0 (may be taken to be infinity) is a limit point of the domain, then the sequence constitutes an asymptotic scale if for every n,*

$$\phi_{n+1}(z) = o(|\phi_n(z)|) \quad \textit{when} \quad z \to z_0.$$

In other words, a sequence of functions is an asymptotic scale if each function in the sequence grows strictly slower (in the limit $z \to z_0$) than the preceding function.

If f is a continuous function on the domain of the asymptotic scale, then f has an asymptotic expansion of order N with respect to the scale as a formal series

$$f(z) \sim \sum_{n=0}^{N-1} a_n \phi_n(z),$$

for some coefficients a_n, if

$$f(z) - \sum_{n=0}^{N-1} a_n \phi_n(z) = O\left(|\phi_N(z)|\right), \quad \textit{when} \quad z \to z_0.$$

3.1. Laplace method. Steepest descent (or 'saddle-point') integration is a method for dealing with integrals of the following type

$$I_N[f,g] = \int_\Omega g(\boldsymbol{x})\, \mathrm{e}^{-Nf(\boldsymbol{x})}\, \mathrm{d}\,\boldsymbol{x}$$

with $\Omega \subseteq \mathbb{R}^n$, $f(\boldsymbol{x})$ and $g(\boldsymbol{x})$ continuous, of which f is bounded from below and g is N-independent, and with $N \in \mathbb{N}$ positive and large. We first take $f(\boldsymbol{x})$ to be real-valued; this is the simplest case, for which finding the asymptotic analysis of I_N goes back to Laplace. We assume that $f(\boldsymbol{x})$ can be expanded in a Taylor series around its (assumed unique) minimum $f(\boldsymbol{x}^\star)$ with $\boldsymbol{x}^\star \in \Omega$, i.e.

$$f(\boldsymbol{x}) = f(\boldsymbol{x}^\star) + \frac{1}{2}\left\langle \boldsymbol{x} - \boldsymbol{x}^\star, \boldsymbol{H}^f(\boldsymbol{x}^\star)\,(\boldsymbol{x} - \boldsymbol{x}^\star)\right\rangle + O(\|\boldsymbol{x} - \boldsymbol{x}^\star\|^3),$$

where

$$\boldsymbol{H}^f(\boldsymbol{x}^\star) \coloneqq \mathrm{Hess}_{\boldsymbol{x}^\star}(f) = \left(\frac{\partial^2 f}{\partial x_i \partial x_j}\right)\Bigg|_{\boldsymbol{x}=\boldsymbol{x}^\star}$$

is the local $n \times n$ curvature matrix and, by hypothesis, $\boldsymbol{H}^f(\boldsymbol{x}^\star) > 0$ being $\boldsymbol{x}^\star$ a minimum. If the integral I_N exists for every $N > N_0$, for some N_0, inserting Taylor expansion into it we obtain

$$I_N[f,g] = \mathrm{e}^{-Nf(\boldsymbol{x}^\star)} \int_\Omega g(\boldsymbol{x})\, \mathrm{e}^{-\frac{1}{2}N\left\langle \boldsymbol{x}-\boldsymbol{x}^\star, \boldsymbol{H}^f(\boldsymbol{x}^\star)(\boldsymbol{x}-\boldsymbol{x}^\star)\right\rangle + O\left(N\|\boldsymbol{x}-\boldsymbol{x}^\star\|^3\right)}\, \mathrm{d}\,\boldsymbol{x}$$

One can now see, that the biggest contribution comes from a small neighbourhood of $\boldsymbol{x}^\star$, as if $\boldsymbol{x}$ moves out of it the integrand decreases exponentially. Passing to new variables $\boldsymbol{x} = \boldsymbol{x}^\star + \frac{\boldsymbol{y}}{\sqrt{N}}$ gives

$$I_N[f,g] = N^{-\frac{n}{2}}\, \mathrm{e}^{-Nf(\boldsymbol{x}^\star)} \int_{\Omega'} g\left(\boldsymbol{x}^\star + \frac{\boldsymbol{y}}{\sqrt{N}}\right) \mathrm{e}^{-\frac{1}{2}\left\langle \boldsymbol{y}, \boldsymbol{H}^f(\boldsymbol{x}^\star)\boldsymbol{y}\right\rangle + O\left(N^{-\frac{1}{2}}|\boldsymbol{y}|^3\right)}\, \mathrm{d}\,\boldsymbol{y}.$$

The last Gaussian integral can be approximated to the first order by

$$g(\boldsymbol{x}^\star) \int_{\mathbb{R}^p} \mathrm{e}^{-\frac{1}{2}\left\langle \boldsymbol{y}, \boldsymbol{H}^f(\boldsymbol{x}^\star)\boldsymbol{y}\right\rangle}\, \mathrm{d}\,\boldsymbol{y} = \frac{g(\boldsymbol{x}^\star)\,(2\pi)^{\frac{n}{2}}}{\sqrt{\det \boldsymbol{H}^f(\boldsymbol{x}^\star)}}.$$

This summarizes to

THEOREM 3.1. *Let $f(\boldsymbol{x})$ and $g(\boldsymbol{x})$ be two real-valued continuous functions defined on $\Omega \subseteq \mathbb{R}^n$. Assume that $f(\boldsymbol{x})$ attains its absolute minimum at some internal point $\boldsymbol{x}^\star \in \Omega$. Then the integral*

$$I_N[f,g] = \int_\Omega g(\boldsymbol{x})\, \mathrm{e}^{-Nf(\boldsymbol{x})}\, \mathrm{d}\,\boldsymbol{x},$$

is approximately equal to

$$I_N[f,g] \approx \left(\frac{2\pi}{N}\right)^{\frac{n}{2}} \frac{g(\boldsymbol{x}^\star)}{\sqrt{\det \boldsymbol{H}^f(\boldsymbol{x}^\star)}}\, \mathrm{e}^{-Nf(\boldsymbol{x}^\star)}.$$

From this latter expansion we can obtain two important identities.

$$\begin{aligned} -\lim_{N\to\infty} \frac{1}{N} \ln \int_\Omega \mathrm{e}^{-Nf(\boldsymbol{x})}\, \mathrm{d}\,\boldsymbol{x} &= -\lim_{N\to\infty} \frac{\ln I_N[f,1]}{N} \\ &= f(\boldsymbol{x}^\star) + \lim_{N\to\infty} \left[\frac{n \log N}{2N} - \frac{1}{N} \ln \int_{\Omega'} \mathrm{e}^{-\frac{1}{2}\left\langle \boldsymbol{y}, \boldsymbol{H}^f(\boldsymbol{x}^\star)\boldsymbol{y}\right\rangle + O\left(N^{-\frac{1}{2}}|\boldsymbol{y}|^3\right)}\, \mathrm{d}\,\boldsymbol{y} \right] \\ &= f(\boldsymbol{x}^\star) = \min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x}). \end{aligned}$$

Second, for ratios of such integrals one finds that

$$\begin{aligned} \lim_{N\to\infty} \frac{\int_\Omega g(\boldsymbol{x})\, \mathrm{e}^{-Nf(\boldsymbol{x})}\, \mathrm{d}\,\boldsymbol{x}}{\int_\Omega h(\boldsymbol{x})\, \mathrm{e}^{-Nf(\boldsymbol{x})}\, \mathrm{d}\,\boldsymbol{x}} &= \lim_{N\to\infty} \frac{I_N[f,g]}{I_N[f,h]} \\ &= \lim_{N\to\infty} \left\{ \frac{\int_{\Omega'} g\left(\boldsymbol{x}^\star + \frac{\boldsymbol{y}}{\sqrt{N}}\right) \mathrm{e}^{-\frac{1}{2}\left\langle \boldsymbol{y}, \boldsymbol{H}^f(\boldsymbol{x}^\star)\boldsymbol{y}\right\rangle + O\left(N^{-\frac{1}{2}}|\boldsymbol{y}|^3\right)}\, \mathrm{d}\,\boldsymbol{y}}{\int_{\Omega'} h\left(\boldsymbol{x}^\star + \frac{\boldsymbol{y}}{\sqrt{N}}\right) \mathrm{e}^{-\frac{1}{2}\left\langle \boldsymbol{y}, \boldsymbol{H}^f(\boldsymbol{x}^\star)\boldsymbol{y}\right\rangle + O\left(N^{-\frac{1}{2}}|\boldsymbol{y}|^3\right)}\, \mathrm{d}\,\boldsymbol{y}} \right\} \\ &= \frac{g(\boldsymbol{x})}{h(\boldsymbol{x})}\Big|_{\boldsymbol{x}=\boldsymbol{x}^\star = \arg\min_{\boldsymbol{x}\in\Omega} f(\boldsymbol{x})}. \end{aligned}$$

The situation becomes more complicated when we allow the dimension n of our integration domain to depend on N. Provided the ratio n/N goes to zero sufficiently fast as $N \to \infty$, one can still prove the above identities, but much more care will be needed in dealing with correction terms.

If the function $f(\boldsymbol{x})$ is complex, the correct procedure to be followed is to deform the integration paths in the complex plane (using Cauchy's theorem) such that along the deformed path the imaginary part of the function $f(\boldsymbol{x})$ is constant, and preferably (if possible) zero. One then proceeds using Laplace's argument and finds the leading order in N of our integral in the usual manner by extremisation of the real part of $f(\boldsymbol{x})$. In combination, our integrals will thus again be dominated by an extremum of the (complex) function $f(\boldsymbol{x})$, but since f is complex this extremum need not be a minimum, so that

$$-\lim_{N\to\infty} \frac{1}{N} \log \int_\Omega \mathrm{e}^{-Nf(\boldsymbol{x})}\, \mathrm{d}\,\boldsymbol{x} = \mathrm{extr}_{\boldsymbol{x}\in\Omega}\, f(\boldsymbol{x})$$

☞ The most known example of Laplace method application is an asymptotic expression for Γ function, called Stirling's approximation. We recall that

$$n! = \Gamma(n+1) = \int_0^\infty t^n \, \mathrm{e}^{-t} \, \mathrm{d}\, t.$$

Introducing new variable $t = sn$ we obtain

$$\Gamma(n+1) = n^{n+1} \int_0^\infty s^n \, \mathrm{e}^{-ns} \, \mathrm{d}\, s = n^{n+1} \int_0^\infty \mathrm{e}^{-nf(s)} \, \mathrm{d}\, s,$$

with $f(s) = s - \log s$. Calculating derivatives gives $f'(s) = 1 - s^{-1}$ and $f''(s) = s^{-2}$. One can easily check that $f(0^+) = f(+\infty) = +\infty$ and the global minimum is attained at $s^* = 1$ with $f(s^*) = 1$ and $f''(s^*) = 1$. Then using Laplace theorem we obtain

$$\Gamma(n+1) \approx \sqrt{2\pi n} n^n \, \mathrm{e}^{-n}.$$

Example: The infinite-range Ising model Let us consider n spins $\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_n)$ system, $\sigma_i = \pm 1$, defined by its Hamiltonian

$$H_n(\boldsymbol{\sigma}) = -h \sum_{j=1}^n \sigma_j - \frac{J}{2n} \sum_{j,k=1}^n \sigma_j \sigma_j =: H_n^{(1)}(\boldsymbol{\sigma}) + H_n^{(2)}(\boldsymbol{\sigma}).$$

Let us assume that the probability distribution on the set of configurations is given by Boltzmann-Gibbs distribution, i.e.

$$\mathbb{P}[\boldsymbol{\sigma} = \boldsymbol{\sigma}_0] = \frac{\mathrm{e}^{-\beta H_n(\boldsymbol{\sigma}_0)}}{Z_N(\beta, H, J)}, \qquad Z_N(\beta, H, J) = \sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta H_n(\boldsymbol{\sigma})}.$$

where $Z_N(\beta, H, J)$ is the partition function, introduced to normalise the distribution. In this example we show how to calculate Z using the Hubbard-Stratonovich transformation. We start with rewriting spin-spin interaction part of the Hamiltonian as follows

$$H_n^{(2)}(\boldsymbol{\sigma}) = -\frac{J}{2n} \sum_{j,k=1}^n \sigma_j \sigma_j = -\frac{J}{2n} \left(\sum_{j=1}^n \sigma_j \right)^2.$$

And applying HS transformation one gets

$$\begin{aligned} Z_N(\beta, H, J) &= \sum_{\boldsymbol{\sigma}} \mathrm{e}^{-\beta H_n^{(1)}(\boldsymbol{\sigma}) + \frac{J\beta}{2N} \left(\sum_{j=1}^N \sigma_j \right)^2} \\ &= \sqrt{\frac{n}{2\pi\beta J}} \sum_{\boldsymbol{\sigma}} \mathrm{e}^{\beta H_n^{(1)}(\boldsymbol{\sigma})} \int_{-\infty}^\infty \exp\left\{ -\frac{ny^2}{2J\beta} + y \left(\sum_{j=1}^N \sigma_j \right) \right\} \mathrm{d}\, y \\ &= \sqrt{\frac{n}{2\pi\beta J}} \int_{-\infty}^\infty \mathrm{e}^{-\frac{ny^2}{2J\beta}} \sum_{\boldsymbol{\sigma}} \exp\left\{ (y + \beta h) \left(\sum_{j=1}^N \sigma_j \right) \right\} \mathrm{d}\, y. \end{aligned}$$

Due to a factorization of summation terms we can easily calculate the sum,

$$\sum_{\boldsymbol{\sigma}} \exp\left\{ (y + \beta h) \left(\sum_{j=1}^N \sigma_j \right) \right\} = \prod_{j=1}^N \left[\sum_{\sigma_j = \pm 1} \exp\{ (y + \beta h) \sigma_j \} \right] = \prod_{j=1}^N 2 \cosh(y + \beta h).$$

Combining all the above one gets

$$Z_N(\beta,H,J)=\sqrt{\frac{n}{2\pi\beta J}}\int\limits_{-\infty}^{\infty}\exp\left\{-\frac{ny^2}{2J\beta}+n\log\left(2\cosh\left(y+\beta h\right)\right)\right\}\mathrm{d}\,y$$
$$=\sqrt{\frac{n}{2\pi\beta J}}\int\limits_{-\infty}^{\infty}\exp\left\{-\frac{ng(y)}{\beta J}\right\}\mathrm{d}\,y,$$

where

$$g(y)=\frac{y^2}{2}-J\beta\log\left(2\cosh\left(y+\beta h\right)\right).$$

The last integral can be calculated approximately in the $n\gg 1$ regime by using Laplace method and the answer can be written as

$$Z_N(\beta,H,J)\approx\frac{1}{\sqrt{|g''(y_0)|}}\,\mathrm{e}^{-\frac{n}{\beta J}g(y_0)},$$

where y_0 is a point of a global minimum of $g(y)$.

4. Complex analysis

We have already given definitions involving complex numbers and used their properties in the previous Section. Here we recap some fundamentals about them, starting from the very definitions.

4.1. Arithmetic of complex numbers.

Definition 4.1. *We define complex plane $\mathbb{C}$ as a field of numbers of the form $x+iy$ with $x,y\in\mathbb{R}$ and i being the imaginary unit satisfying $i^2=-1$. $x\equiv\Re z$ is called real part of z and $y\equiv\Im z$ is the imaginary part of z.*

A complex number $z=x+iy$ can be associated with a point $(x,y)\in\mathbb{R}^2$, where x,y are usual (Euclidean) coordinates. In the polar coordinates, every nonzero $z\in\mathbb{C}$ can be defined by a pair (r,θ) where $r=\sqrt{x^2+y^2}$ and θ is defined as $\theta=\arccos\frac{x}{r}$ up to integer multiples of 2π. The numbers r and θ are called, respectively, the *module* and the *argument* of the complex number z, and are denoted by $|z|$ and $\arg z$. A complex number is can be then represented as $z=r\,\mathrm{e}^{i\theta}$. We stress again that the argument is not uniquely defined: one can take $\theta+2\pi k$ with any $k\in\mathbb{Z}$. We can choose $k\in\mathbb{Z}$ in such a way that $-\pi<\theta+2\pi k\leq\pi$. This number $\theta+2\pi k$ is said to be the principal value of the argument and is denoted by $\operatorname{Arg} z$.

Definition 4.2. *For every $z=x+iy=r\,\mathrm{e}^{i\theta}\in\mathbb{C}$ one can define complex conjugate of z as $\overline{z}=x-iy$ or $\overline{z}=r\,\mathrm{e}^{-i\theta}$. Geometrically it corresponds to the reflection over x axis in Euclidean coordinates.*

Observe that

$$z\cdot\overline{z}=|z|^2\in\mathbb{R}_+.$$

Algebraic operations on complex numbers are defined as

$$(x_1+iy_1)+(x_2+iy_2)=(x_1+x_2)+i\left(y_1+y_2\right),$$
$$(x_1+iy_1)\cdot(x_2+iy_2)=(x_1x_2-y_1y_2)+i\left(x_1y_2+x_2y_1\right),$$
$$(x+iy)^{-1}=\frac{x-iy}{x^2+y^2}=\frac{\overline{x+iy}}{|x+iy|^2}.$$

PROPOSITION 4.1 (De Moivre's formula). *For any complex $z = r\,\mathrm{e}^{i\theta} \in \mathbb{C}$ we have*

$$z^n = r^n\,\mathrm{e}^{in\theta} = r^n\left(\cos(n\theta) + i\sin(n\theta)\right).$$

DEFINITION 4.3. *The distance between two complex numbers z_1, z_2 is given by* $\operatorname{dist}(z_1, z_2) = |z_1 - z_2|$.

The distance between two complex numbers is the same as the Euclidean distance between the corresponding Euclidean space representatives. The notion of distance allows to introduce the standard definitions of open and closed sets, convergence of sequences, continuity of functions, etc. Let us just underline that convergence of the sequence $z_n \to z_0$ is equivalent to two convergences $x_n = \Re z_n \to x_0 = \Re z_0$ and $y_n = \Im z_n \to y_0 = \Im z_0$. Moreover we can define path in $\mathbb{C}$ as follows.

DEFINITION 4.4. *Let z_1, z_2 be two points in complex plane. A path from z_1 to z_2 is a continuous map $\gamma : [0,1] \to \mathbb{C}$ such that $\gamma(0) = z_1$ and $\gamma(1) = z_2$.*

4.2. Functions of complex arguments. A *complex function* is any function $f : \mathbb{C} \to \mathbb{C}$. Any complex function can be considered as a map $\mathbb{R}^2 \to \mathbb{R}^2$ and decomposed as $f(x,y) = u(x,y) + iv(x,y)$, where $u = \Re f$, $v = \Im f$ and both $u, v\colon \mathbb{R}^2 \to \mathbb{R}$ are two real valued functions of two real variables. A complex function f is continuous iff its real and imaginary parts are continuous functions.

EXAMPLE Complex exponent is defined by $\mathrm{e}^z = \mathrm{e}^{x+iy} = \mathrm{e}^x(\cos y + i\sin y)$.

EXAMPLE To define complex logarithm one should solve equation $\mathrm{e}^w = z$. Let $z = x+iy$ and $w = u + iv$. Then equating real and imaginary parts one has

$$\begin{cases} \mathrm{e}^u \cos v &= x, \\ \mathrm{e}^u \sin v &= y, \end{cases}$$

and one can conclude that

$$\begin{cases} u &= \log|z|, \\ v &= \arg z. \end{cases}$$

However, $\arg z$ is a multi-valued function and so is a logarithm. One can get a single-valued function by taking principal value

$$\operatorname{Log} z \coloneqq \log|z| + i\operatorname{Arg} z.$$

Let us now review some results about differentiability of complex functions.

DEFINITION 4.5. *A complex function $f(z)$ is called differentiable at point z_0 if there exists a number $\partial_z f(z_0) \in \mathbb{C}$ such that*

$$f(z_0 + \Delta z) = f(z_0) + \partial_z f(z_0)\Delta z + O(|\Delta z|^2), \text{ when } \Delta z \to 0.$$

Taking real and imaginary parts of the last identity we obtain

$$\begin{cases} u(x_0 + \Delta x, y_0 + \Delta y) - u(x_0, y_0) &= \partial_x u \Delta x + \partial_y u \Delta y + O\left((\Delta x)^2 + (\Delta y)^2\right), \\ v(x_0 + \Delta x, y_0 + \Delta y) - v(x_0, y_0) &= \partial_x v \Delta x + \partial_y v \Delta y + O\left((\Delta x)^2 + (\Delta y)^2\right), \end{cases}$$

Comparing with

$$f(z_0 + \Delta z) - f(z) = \partial_z f \Delta z = (\partial_x u + i\partial_x v)\Delta x + (-i\partial_y u + \partial_y v) i\Delta y + O(|\Delta z|^2)$$

that implies

$$\partial_x u = \partial_y v \qquad -\partial_y u = \partial_x v.$$

The equations above are called *Cauchy–Riemann equations* and are necessary condition for differentiability of f. Conversely, it can be shown that this condition is also sufficient provided that the partial derivatives of u and v are continuous.

THEOREM 4.2 (Cauchy–Riemann equations). *Let $f(z) = u(x,y) + iv(x,y)$ be a complex function. Then f is differentiable at the point $z_0 = x_0 + iy_0$ if real functions of two variables u and v are differentiable and their partial derivatives are continuous and satisfy Cauchy–Riemann equations*

$$\partial_x u(x_0,y_0) = \partial_y v(x_0,y_0), \quad -\partial_y u(x_0,y_0) = \partial_x v(x_0,y_0).$$

In this case $\partial_z f(z_0) = \partial_x u(x_0,y_0) + i\partial_x v(x_0,y_0)$.

Sometimes the Cauchy–Riemann equations are written as $\partial_{\bar z} f(z_0) = 0$. This suggests that f can not depend on $\overline{z}$ to be differentiable.

EXAMPLE Let us take $f(z) = z^2 = \left(x^2 - y^2\right) + 2ixy$. Then

$$\partial_x u = 2x \qquad \partial_y v = 2x \qquad \partial_y u = -2y \qquad \partial_x v = 2y.$$

Cauchy–Riemann equations are satisfied and therefore

$$\partial_z f(z) = 2x + i2y = 2z,$$

as one should expect.

EXAMPLE Let us take $f(z) = \mathrm{e}^z = \mathrm{e}^x \cos y + i\,\mathrm{e}^x \sin y$. Then

$$\partial_x u = \mathrm{e}^x \cos y, \qquad \partial_y v = \mathrm{e}^x \cos y, \qquad \partial_y u = -\,\mathrm{e}^x \sin y, \qquad \partial_x v = \mathrm{e}^x \sin y.$$

Cauchy–Riemann equations are satisfied and therefore

$$\partial_z f(z) = \mathrm{e}^x \cos y + i\,\mathrm{e}^x \sin y = \mathrm{e}^z,$$

as one should expect.

EXAMPLE Let us take $f(z) = \left|z^2\right| = x^2 + y^2$. One should expect that $f(z)$ is not differentiable in $\mathbb{C} \setminus \{0\}$, because $\partial_{\bar z} f(z) = z$. Cauchy–Riemann equations take the form

$$\partial_x u = 2x = \partial_y v = 0, \qquad \partial_y u = 2y = -\partial_x v = 0,$$

that gives $x = y = 0$. So $|z|^2$ is differentiable only at the origin.

One can see, that differentiability is a local property and unlikely to the real case does not yield any differentiability even in a close neighbourhood.

DEFINITION 4.6. *We say that $D \subset \mathbb{C}$ is a domain if D is open and connected.*

DEFINITION 4.7. *We say that the function f is holomorphic in a neighbourhood U of z_0 if it is differentiable everywhere in U. We say that the function f is holomorphic in a domain D if it is differentiable everywhere in D. We say that a function is entire if it is holomorphic in the whole complex plane.*

We denote the set of holomorphic function on D as $H(D)$. It is important to realise that being holomorphic, unlike differentiability, is not a property of a function at a point, but on an open set of points. The reason for this is to able to

eliminate from the class of interesting functions, functions which may be differentiable at a point but nowhere else. Surprisingly, holomorphic functions have even better smoothness than just differentiability. More precisely

THEOREM 4.3. *Let $f(z)$ be holomorphic in domain $D \subseteq \mathbb{C}$. Then $\partial_z f(z)$ is continuous in D and f has all higher continuous derivatives in D.*

The theorem says that f only needs to have a first derivative on D for this to hold – remarkably, the continuity of that derivative and the existence and continuity of all the higher derivatives, all then follow for free. Infinitely differentiable real valued functions in a ball can be represented in Taylor series: the same holds for complex functions.

4.2.1. *Complex series.* Let $w_0, w_1, w_2, \ldots$ be a sequence of complex numbers. As in the real case, we say that the (formal) infinite series

$$S = \sum_{k=0}^{\infty} w_k$$

converges if the sequence of its partial sums $S_n = \sum_{k=0}^{n} w_k$ converges to a limit $w \in \mathbb{C}$ as $m \to \infty$. If this is the case, we write $w = \sum_{k=0}^{\infty} w_k$ and call w the sum of the series; we may indicate the series more briefly by $\sum_k w_k$, and write $\sum_k w_k < \infty$ to indicate a convergent series and $\sum_k w_k = \infty$ to indicate a divergent series.

EXAMPLE $\sum_k \alpha^k$ is convergent if $|\alpha| < 1$ and divergent if $|\alpha| > 1$.

PROPOSITION 4.4. *For any complex power series $\sum_{n=0}^{\infty} a_n (z - z_0)^n$ there is a value $R \geq 0$ such that, if $R \neq 0$, then the series converges absolutely for those $z \in \mathcal{B}(z_0, R)$, and diverges for $|z - z_0| > R$. If $R = \infty$ then the series converges absolutely for all $z \in \mathbb{C}$. If $R = 0$ then the series is divergent for all $z \neq 0$. The radius of convergence is given by*

$$R = \left(\limsup_k |a_k|^{\frac{1}{k}} \right)^{-1}.$$

As in the real case, the lemma says nothing about the behaviour of the series for $|z - z_0| = R$. This depends on finer properties of the coefficients a_n; the series may diverge or converge at those points.

DEFINITION 4.8. *f is said to be complex analytic in domain D if it is infinitely times differentiable at every point of D and for each $z_0 \in D$ there is an open disc $\mathcal{B}(z_0, R) \subset D$ in which*

$$f(z) = \sum_{k=0}^{\infty} \frac{f^{(k)}(z_0)}{k!} (z - z_0)^k.$$

THEOREM 4.5. *Let D be a domain in $\mathbb{C}$ and f holomorphic on it. Then f is complex analytic in D.*

Finally, let us mention a realtion, due to the Cauchy–Riemann equations, between harmonic functions and holomorphic functions.

DEFINITION 4.9. *Let $u\colon D \subseteq \mathbb{R}^2 \to \mathbb{R}$ be a twice differentiable function defined on a domain D. It is called harmonic function if u solves the Laplace equation on D*

$$\Delta u\,(x,y) = \left(\partial_x^2 + \partial_y^2\right) u = 0, \quad (x,y) \in D.$$

THEOREM 4.6. *Let $f(z)$ be a holomorphic function in domain $D \subseteq \mathbb{C}$. Then its real and imaginary parts are harmonic functions in D.*

Exercises

(1) Show that the alternating harmonic series $\sum_{n=1}^{\infty} \frac{(-1)^n}{n}$ is convergent.
(2) Find the radius and a ball of convergence for the following power series
   (a) $\sum_{k=0}^{\infty} \frac{k!^2}{(2k)!} x^k$.
   (b) $\sum_{k=0}^{\infty} \frac{x^k}{\sin^k k}$.
   (c) $\sum_{k=0}^{\infty} \frac{\left(2+(-1)^k\right)^k}{k} (x-\pi)^k$.
(3) Find Taylor series expansion for the following functions and calculate corresponding radius of convergence
   (a) $f(x) = \sin x$ around $x = \frac{\pi}{2}$.
   (b) $\ln(1+x)$ around the origin.
   (c) $f(x) = \arctan x$ around the origin. *Hint:* start with the Taylor series for $f'(x)$.
   (d) $f(x) = \frac{1-\cos x}{x^2}$ around $x = 0$. *Hint:* write the series for $\cos x$ first.
(4) Prove Eq. (8) for $n = 1$, assuming $A > 0$ and $b \in \mathbb{R}$. *Hint:*for the first integral consider it squared and in corresponding double integral perform change to polar coordinates. In the second integral complete the square and make corresponding change of variables to get previous integral.
(5) Prove Eq. (9) for any real symmetric, positive matrix $\boldsymbol{A} \in \mathcal{M}_{n\times n}\mathbb{R}$ and arbitrary vector $\boldsymbol{b} \in \mathbb{R}^n$. *Hint:* Use spectral decomposition of matrix $\boldsymbol{A}$, change integration variables accordingly to reduce the problem to diagonal matrix $\boldsymbol{A}$. In the second integral perform linear change of variables to kill a linear term and then use the first integral value.
(6) Let $\Gamma(M,a)$ denotes upper incomplete Γ-function defined by

$$\Gamma(x,a) = \int_a^{\infty} \mathrm{e}^{-t}\, t^{x-1}\, \mathrm{d}\, t.$$

Using Laplace method for asymptotic analysis of integrals depending on a big parameter show that
   (a) the following limit holds

$$\lim_{x\to\infty} \frac{\Gamma(x-1,ax)}{\Gamma(x-1)} = \begin{cases} 1, & 0 \le a < 1, \\ \frac{1}{2}, & a = 1 \\ 0, & \text{otherwise.} \end{cases}$$

   (b) for large x and $a > 1$ one has asymptotically

$$\frac{\Gamma(x-1,ax)}{\Gamma(x-1)} \approx \frac{1}{\sqrt{2\pi x}} \frac{1}{a\,(a-1)}\, \mathrm{e}^{-x(a-1-\ln a)}.$$

(7) Show that $f(z) = z^n$ is an entire function and prove its derivative is given by $f'(z) = nz^{n-1}$.

LECTURE 3

Calculus (continue)

1. Integration along a contour in complex plane

In this chapter we will consider the fundamental problem of integration along a curve in the complex plane. In particular, we would like to make sense out of something like

$$\int_{\gamma} f(z)\,\mathrm{d}\,z$$

where γ is a *contour* in $\mathbb{C}$. We have given the definition of path above. Here it is convenient to give few additional ones to specify the type of objects we will deal with.

DEFINITION 1.1. *A path between z_0 and z_1 in the complex plane is said to be simple if it does not cross itself (that is, $\gamma(t_1) \neq \gamma(t_2)$ for $t_1 \neq t_2 \in (0,1)$. If $\gamma(0) = \gamma(1)$ the path is s.t.b. closed. A path is said to be smooth (or continuously differentiable) if the derivative $\dot{\gamma}(t) \coloneqq \partial_t \gamma(t)$ exists and is continuous, using the left derivative at the point z_0 and the right at z_1.*

DEFINITION 1.2. *A contour is a piecewise smooth path, i.e., a path $\gamma : [0,1] \to \mathbb{C}$ for which there exists a finite collection of numbers $0 = \tau_0 < \tau_1 < \ldots < \tau_{n-1} < \tau_n = 1$ such that $\gamma : [\tau_k, \tau_{k+1}] \to \mathbb{C}$ are smooth paths.*

PROPOSITION 1.1. *The length of a contour γ is given by*

$$l(\gamma) = \int_0^1 |\dot{\gamma}(t)|\,\mathrm{d}\,t.$$

DEFINITION 1.3 (Contour integral). *Let $\gamma : [0,1] \to \mathbb{C}$ be a smooth path and f be a continuous complex function on a neighbourhood of $\gamma([0,1])$. Then*

$$\int_{\gamma} f(z)\,\mathrm{d}\,z = \int_0^1 f(\gamma(t))\,\dot{\gamma}(t)\,\mathrm{d}\,t.$$

If γ is a contour composed of smooth paths $\gamma_k : [\tau_{k-1}, \tau_k] \to \mathbb{C}$ with $k = 1, \ldots, n$ then

$$\int_{\gamma} f(z)\,\mathrm{d}\,z = \sum_{k=1}^{n} \int_{\tau_{k-1}}^{\tau_k} f(\gamma(t))\,\dot{\gamma}_k(t)\,\mathrm{d}\,t.$$

If the contour is closed we will write $\oint_{\gamma} f(z)\,\mathrm{d}\,z$ to emphasize this fact.

PROPOSITION 1.2. *If f is differentiable and its derivative f' is continuous along the contour $\gamma : [0,1] \to \mathbb{C}$, then*

$$\int_\gamma f'(z)\,\mathrm{d}\,z = f\left(\gamma(1)\right) - f\left(\gamma(0)\right).$$

DEFINITION 1.4. *Let f be a complex function defined on an open set $D \subset \mathbb{C}$. A function F defined on the same set D is said to be a primitive of f if F is holomorphic in D and $F'(z) = f(z)$ for all $z \in D$.*

COROLLARY 1.3. *If f has a primitive $F \in H(D)$, then*

$$\int_\gamma f(z)\,\mathrm{d}\,z = F\left(\gamma(1)\right) - F\left(\gamma(0)\right).$$

In particular, if γ is a closed contour then

$$\oint_\gamma f(z)\,\mathrm{d}\,z = 0.$$

EXAMPLE Let γ_r be the anticlockwise oriented circle about z_0 of radius r. We want to calculate

$$I(z) = \frac{1}{2\pi i}\oint_{\gamma_r} \frac{1}{w-z}\,\mathrm{d}\,w,$$

for z lying in the open disc $B(z_0, r)$ bounded by γ_r. Let $z = s\,\mathrm{e}^{i\theta}$, where $s < r$ and $\theta \in (-\pi, \pi]$. We can parametrize contour as

$$\gamma(t) = r\,\mathrm{e}^{i(2\pi t+\theta)}, \quad t \in (0,1].$$

Then by definition

$$I(z) = \int_0^1 \frac{r\,\mathrm{e}^{2\pi i t+i\theta}}{s\,\mathrm{e}^{i\theta} - r\,\mathrm{e}^{i\theta+2\pi i t}}\,\mathrm{d}\,t = \int_0^1 \frac{1}{\frac{s}{r}\,\mathrm{e}^{-2\pi i t} - 1}\,\mathrm{d}\,t = \cdots = 1.$$

THEOREM 1.4 (Cauchy's integral formula). *Assume that $f \in H\left(\mathcal{B}(z_0, R)\right)$. Let $r < R$ and γ_r be the anticlockwise oriented circle around z_0 of radius r. Then*

$$f(z) = \frac{1}{2\pi i}\oint_{\gamma_r} \frac{f(w)}{w-z}\,\mathrm{d}\,w, \quad \forall z \in \mathcal{B}(z_0, r).$$

THEOREM 1.5. *Assume that $f \in H\left(\mathcal{B}(z_0, R)\right)$. Let $r < R$ and γ_r be the anticlockwise oriented circle around z_0 of radius r. Then*

$$f(z) = \sum_{k=0}^{\infty} c_k \left(z - z_0\right)^k, \quad \forall z \in \mathcal{B}(z_0, r),$$

where

$$c_k = \frac{1}{2\pi i}\oint_{\gamma_r} \frac{f(w)}{\left(w - z_0\right)^{k+1}}\,\mathrm{d}\,w,$$

and the series is absolutely and uniformly convergent in the disc $\mathcal{B}(z_0, r)$.

COROLLARY 1.6. *With the assumptions of the theorem, the n-th derivative $f^{(n)}$ satisfies*

$$f^{(n)}(z) = \frac{n!}{2\pi i} \oint_{\gamma_r} \frac{f(w)}{(w-z)^{n+1}} \, \mathrm{d}\, w, \quad \forall z \in \mathcal{B}(z_0, r).$$

1.1. Isolated singularities and residues. Below we extend our class of holomorphic functions to consider functions with 'mild' singularities.

DEFINITION 1.5. *We shall say that $f(z)$ has an isolated singularity at the point $z = z_0$ if f is holomorphic in a punctured disc $\dot{\mathcal{B}}(z_0, r) \coloneqq \mathcal{B}(z_0, r) \setminus \{z_0\}$ for some $r > 0$ but is not holomorphic at z_0.*

EXAMPLE $f(z) = 1/z$ has an isolated singularity at 0.

DEFINITION 1.6. *Assume that f has an isolated singularity at $z = z_0$. Then there are three possibilities:*

1. *the limit $\lim_{z \to z_0} |f(z)|$ exists as a finite real number. In this case we say that f has a removable singularity at z_0;*
2. *$\lim_{z \to z_0} |f(z)| = \infty$. In this case we say that f has a pole at z_0;*
3. *the limit $\lim_{z \to z_0} |f(z)|$ does not exist as a finite real number or ∞. In this case we say that f has an essential singularity at z_0.*

DEFINITION 1.7. *Let f be a holomorphic function in the complement of a disc about the origin. We shall say that f is bounded at infinity if $f(1/z)$ has a removable singularity at $z = 0$.*

EXAMPLE The function $f(z) = \frac{\sin z}{z}$ has a removable singularity at the origin.
The function $f(z) = \frac{1}{z}$ has a pole at the origin.
The function $f(z) = \mathrm{e}^{-\frac{1}{z}}$ has an essential singularity at the origin.

DEFINITION 1.8. *A complex function on domain D is called meromorphic if it is holomorphic in D except for a set of poles. Note that the pole set of a meromorphic function is discrete (but may be infinite).*

There is a simple yet useful generalisation of the notion of power series which can handle the case of meromorphic functions, that are, in a sense, "almost holomorphic". These series are known as *Laurent* series and consist of a sum of two power series.

DEFINITION 1.9. *A Laurent series about the point z_0 is a sum of two power series one consisting of positive powers of $z - z_0$ and the other of negative powers:*

$$\sum_{k=0}^{\infty} c_k (z - z_0)^k + \sum_{k=1}^{\infty} c_{-k} (z - z_0)^{-k} =: \sum_{k=-\infty}^{\infty} c_k (z - z_0)^k.$$

A Laurent series is said to converge if each of the two power series converges. The first series, being a power series in $z - z_0$ converges inside some disc of convergence $\mathcal{B}(z_0, R)$ for some $0 \leq R \leq \infty$. The second series, however, is a power series in $w = \frac{1}{z - z_0}$. Hence it will converge inside a circle of convergence $|w| \leq R_0$, that

is, for $|z-z_0| > \frac{1}{R_0} =: r$. In other words, such a Laurent series will converge in an *annulus* $r < |z-z_0| < R$. For this to make sense, we need $r < R$: if this is not the case, then the Laurent series does not converge anywhere. One can easily see that if a Laurent series is convergent in an annulus, then it is holomorphic inside of it. Therefore we can expect that any holomorphic in annulus function could be decomposed in a Laurent series, that will converge to the function.

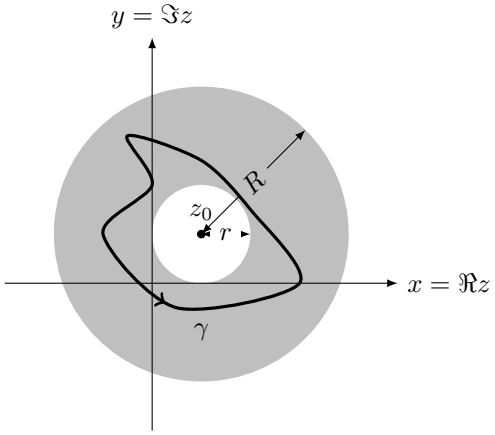
THEOREM 1.7 (Laurent's expansion). *Let $0 \le r < R \le \infty$ and $D(z_0; r, R)$ be the open annulus $r < |z-z_0| < R$. If f is holomorphic in $D(z_0; r, R)$ then there exist a set of complex numbers $\{c_k\}_{k=-\infty}^{\infty}$ such that*

$$f(z) = \sum_{k=-\infty}^{\infty} c_k (z-z_0)^k,$$

for all $z \in D(z_0; r, R)$, where the series is absolutely and uniformly convergent on any annulus $D(z_0; R_1, R_2)$ with $r < R_1 < R_2 < R$. Moreover the coefficients of the Laurent series are given by

$$c_k = \frac{1}{2\pi i} \int_{\gamma} \frac{f(\zeta)}{(\zeta - z_0)^{k+1}} \, \mathrm{d}\zeta,$$

where γ is any positively oriented loop lying in the annulus and containing z_0 in its interior.



If $r = 0$ then function f is holomorphic in $\mathcal{B}(z_0, R)$ and can be rewritten as a Taylor series. This is consistent with Laurent expansion as integrals of the form

$$\int_{\Gamma} \frac{f(\zeta)}{(\zeta - z_0)^{k+1}} \, \mathrm{d}\zeta,$$

vanish for $k < 0$ as integrals of holomorphic functions over a closed contour.

EXAMPLE Let us build Laurent expansion for $f(z) = \frac{z^2-2z+3}{z-2}$ around $z = 1$ in the region $|z-1| > 1$. The direct way to proceed is by computing

$$c_k = \frac{1}{2\pi i} \int_{|\zeta-1|=2} \frac{f(\zeta)}{(\zeta-1)^{k+1}} \, \mathrm{d}\zeta.$$

However, for algebraic functions it is more convenient to do a direct manipulation. Let us introduce $w = z - 1$ with $|w| > 1$. Then

$$f(z) = \frac{w^2+2}{w-1} = \left(w + \frac{2}{w}\right)\frac{1}{1-\frac{1}{w}} = \left(w + \frac{2}{w}\right)\sum_{k=0}^{\infty} w^{-k} = \sum_{k=-\infty}^{1} w^k + 2\sum_{k=-\infty}^{-1} w^k = w + 1 + 3\sum_{k=-\infty}^{-1} w^k = (z-1) + 1 + \sum_{k=0}^{\infty} \frac{3}{(z-1)^{k+1}}. \tag{10}$$

Laurent expansion obviously depends on the centre of an annulus. In the next example we would like to stress the fact, that by taking different annulus one also gets different Laurent expansion for the same function and the same center.

EXAMPLE Let us build Laurent expansion for $f(z) = \frac{1}{z^2-3z+2}$ in three different regions

(1) $\Omega_1 = \{z : |z| < 1\}$;
(2) $\Omega_2 = \{z : 1 < |z| < 2\}$;
(3) $\Omega_3 = \{z : |z| > 2\}$.

We start by decomposing the function into partial fractions

$$f(z) = \frac{1}{z-2} - \frac{1}{z-1}.$$

In region Ω_1 we have

$$f(z) = -\frac{1}{2}\cdot\frac{1}{1-\frac{z}{2}} + \frac{1}{1-z} = -\frac{1}{2}\sum_{k=0}^{\infty}\left(\frac{z}{2}\right)^k + \sum_{k=0}^{\infty} z^k = \sum_{k=0}^{\infty}\left(1 - 2^{-k-1}\right) z^k.$$

In region Ω_2 we have

$$f(z) = -\frac{1}{2}\cdot\frac{1}{1-\frac{z}{2}} - \frac{1}{z}\cdot\frac{1}{1-\frac{1}{z}} = -\frac{1}{2}\sum_{k=0}^{\infty}\left(\frac{z}{2}\right)^k - \frac{1}{z}\sum_{k=0}^{\infty} z^{-k} = -\sum_{k=0}^{\infty} 2^{-k-1} z^k - \sum_{k=1}^{\infty} z^{-k}.$$

Finally in region Ω_3 we have

$$f(z) = \frac{1}{z}\cdot\frac{1}{1-\frac{2}{z}} - \frac{1}{z}\cdot\frac{1}{1-\frac{1}{z}} = \frac{1}{z}\sum_{k=0}^{\infty}\left(\frac{2}{z}\right)^k - \frac{1}{z}\sum_{k=0}^{\infty} z^{-k} = \sum_{k=1}^{\infty}\left(2^{k-1} - 1\right) z^{-k}.$$

DEFINITION 1.10. *If $f(z)$ has an isolated singularity in $z = z_0$ (i.e. it is analytic for $0 < |z - z_0| < \epsilon$ for some small ϵ but not in z_0), and the singularity can be written as*

$$f(z) = \frac{c_{-m}}{(z-z_0)^m} + \ldots + \frac{c_{-1}}{(z-z_0)} + \phi(z) \qquad 0 < |z - z_0| < \epsilon,$$

with $\phi(z)$ analytic at $|z - z_0| < \epsilon$, then we say that $f(z)$ has a pole of order m at $z = z_0$ (if $m = 1$, for example, it is called a simple pole). We define the residue of f at $z = z_0$ as

$$\operatorname{Res}(f, z_0) = c_{-1}.$$

In some case it is simple to compute the residue in a point

(1) Assume that $f(z)$ has a *simple pole* at $z = z_0$, i.e., $f(z) = c_{-1}(z - z_0)^{-1} + \sum_{k=0}^{\infty} c_k (z - z_0)^k$. Then
$$\operatorname{Res}(f, z_0) = \lim_{z \to z_0} (z - z_0) f(z).$$

(2) If $f(z)$ has a *pole of order* m at $z = z_0$, then $g(z) \coloneqq (z - z_0)^m f(z) = \sum_{k=0}^{\infty} c_{k-m} (z - z_0)^k$, from which we have to extract the coefficient of $(z - z_0)^{m-1}$. But this is given by
$$\operatorname{Res}(f, z_0) = c_{-1} = \frac{g^{(m-1)}(z_0)}{(m-1)!} = \frac{1}{(m-1)!} \lim_{z \to z_0} \partial_z^{m-1} \left[(z - z_0)^m f(z) \right].$$

(3) Finally, if
$$f(z) = \frac{\phi(z)}{h(z)} \quad \text{with } \phi(z), h(z) \text{ analytic at } z = z_0$$
and $h(z_0) = 0$ but $h'(z_0) \neq 0$, then f has a simple pole at $z = z_0$ and
$$\operatorname{Res}(f, z_0) = \lim_{z \to z_0} (z - z_0) \frac{\phi(z)}{h(z)} = \frac{\phi(z_0)}{h'(z_0)}.$$

EXAMPLE Let us find all isolated singularities of $f(z) = \cot z^2 = \frac{\cos z^2}{\sin z^2}$ and corresponding residues. The function f has singularities only at points where $\sin z^2 = 0$, i.e., for $z = \pm\sqrt{\pi k}$ and $z = \pm i\sqrt{\pi k}$ for $k \in \mathbb{N}$. At every such a point, except $z = 0$, $\partial_z \left(\sin z^2\right) = 2z \cos z^2 \neq 0$, and therefore we can apply the last result and compute
$$\operatorname{Res}\left(f, \pm\sqrt{\pi k}\right) = \frac{\cos \pi k}{\pm 2\sqrt{\pi k} \cos \pi k} = \pm \frac{1}{2\sqrt{\pi k}},$$
$$\operatorname{Res}\left(f, \pm i\sqrt{\pi k}\right) = \frac{\cos(-\pi k)}{\pm 2i\sqrt{-\pi k} \cos(-\pi k)} = \pm \frac{1}{2i\sqrt{\pi k}}.$$
For $z = 0$ we have $\sin z^2 = 0$ and $\partial_z \left(\sin z^2\right)|_{z=0} = 0$ while $\partial_z^2 \left(\sin z^2\right)|_{z=0} = 2 \neq 0$. As a consequence
$$\operatorname{Res}(f, 0) = \lim_{z \to 0} \partial_z \left[\frac{z^2 \cos z^2}{\sin z^2} \right] = \lim_{z \to 0} \frac{\sin z^2 \left(2z \cos z^2 - 2z^3 \sin z^2\right) - 2z^3 \cos^2 z^2}{\sin^2 z^2} = 0.$$

The crucial importance of residues is motivated by the following theorem.

THEOREM 1.8 (Cauchy Residue theorem). *Let γ be a closed simple contour in $\mathbb{C}$ and $f : \mathbb{C} \to \mathbb{C}$ analytic along γ and its interior except possibly at a finite number of points $z_1, \ldots, z_m$, at which points $f(z)$ has isolated singularities. Then, with γ being oriented in an anti-clockwise sense*
$$\oint_\gamma f(z) \, \mathrm{d}\, z = 2\pi i \sum_{k=1}^{m} \operatorname{Res}(f, z_k).$$

DEFINITION 1.11 (Residue at infinity). *Let $f : \mathbb{C} \to \mathbb{C}$ be an analytic function in $\mathbb{C}$ except possibly at a finite number of points $z_1, \ldots, z_m$ at which points $f(z)$ has isolated singularities. Given a simple closed contour γ oriented in an anti-clockwise sense containing all singularities in its interior, we define the residue at infinity by*
$$\operatorname{Res}(f, \infty) = -\frac{1}{2\pi i} \oint_\gamma f(z) \, \mathrm{d}\, z.$$

PROPOSITION 1.9. *The residue* $\operatorname{Res}(f,\infty)$ *can be calculated as a residue of* $g(z) = -\frac{1}{z^2} f\left(1/z\right)$ *at zero.*

Cauchy's theorem can be reformulated as follows.

PROPOSITION 1.10. *The sum of all residues for any function* f *with finitely many isolated singularities in* $\{z_i\}_{i=1}^m$ *is equal to* 0*, i.e.*

$$\sum_{k=1}^{m} \operatorname{Res}(f, z_k) + \operatorname{Res}(f,\infty) = 0.$$

EXAMPLE Let us compute an integral

$$I = \oint_\gamma \frac{z^2+3z+2}{(z^4-1)(z-1)^2}\,\mathrm{d}\,z,$$

where γ is a circle with centre at the origin of radius 2. To calculate the integral first we would like to find all the singularities of the integrand. These are all zeros of the denominator, i.e. $z = \pm 1, \pm i$ and they all lie inside of the contour. At $z=-1$ we have removable singularity, and we don't consider it. At $z = \pm i$ we have first order poles with residues

$$\operatorname{Res}(f,i) = \lim_{z\to i}(z-i)f(z) = \lim_{z\to i}\frac{z^2+3z+2}{(z+i)(z^2-1)(z-1)^2} = -\frac{1}{8} - \frac{3}{8}i,$$

$$\operatorname{Res}(f,-i) = \lim_{z\to -i}(z+i)f(z) = \lim_{z\to -i}\frac{z^2+3z+2}{(z-i)(z^2-1)(z-1)^2} = -\frac{1}{8} + \frac{3}{8}i.$$

At $z=1$ there is a pole of the third order and

$$\operatorname{Res}(f,1) = \lim_{z\to 1}\partial_z^2 (z-2)^3 f(z) = \lim_{z\to 1}\partial_z^2 \frac{z+2}{(z^2+1)} = \ldots = \frac{1}{2}.$$

Combining all the above we obtain

$$I = \frac{\pi i}{4}.$$

EXAMPLE Let us calculate an integral

$$I = \oint_\gamma z\,\mathrm{e}^{1/z}\,\mathrm{d}\,z,$$

where γ is the unit circle centered in the origin. There is exactly one isolated singularity inside of a unit circle. However, it is an essential singularity and we want to omit calculation of a residue at it. This can be done by using residue at infinity:

$$I = -2\pi i \operatorname{Res}(f,\infty).$$

The residue can be calculated as a residue at the origin for

$$g(z) = -\frac{1}{z^2} f\left(\frac{1}{z}\right) = -\frac{1}{z^3}\,\mathrm{e}^z = -\frac{1}{z^3} - \frac{1}{z^2} - \frac{1}{2!z} - \ldots,$$

where for the last identity we used Taylor series expansion for e^z. Therefore,

$$\operatorname{Res}(g,0) = -\frac{1}{2},$$

and

$$I = \pi i.$$

1.2. Applications of Cauchy Residue theorem. There are many applications of the residue theorem to evaluate *real integrals and to summing infinite series*. The first application of such a kind we would like to discuss is a calculation of trigonometric integrals of the form

$$\int_0^{2\pi} Q\left(\cos\theta, \sin\theta\right) \mathrm{d}\,\theta,$$

where $Q\left(\bullet, \bullet\right)$ is a rational function. In this case we introduce $z = \mathrm{e}^{i\theta}$ and change $\cos\theta = \frac{z+z^{-1}}{2}$, $\sin\theta = \frac{z-z^{-1}}{2i}$ and $\mathrm{d}\,\theta = \frac{\mathrm{d}\,z}{iz}$ to obtain a rational function integral along the unit circle.

EXAMPLE Let us calculate

$$I = \int_0^{2\pi} \frac{\sin^2\theta}{5 + 4\cos\theta}\,\mathrm{d}\,\theta.$$

After performing change of variables we obtain

$$I = -\frac{1}{4i}\oint_\gamma \frac{z^4 - 2z^2 + 1}{z^2\left(2z^2 + 5z + 2\right)}\,\mathrm{d}\,z = -\frac{\pi}{2}\sum_i \operatorname{Res}\left(\frac{z^4 - 2z^2 + 1}{z^2\left(2z^2 + 5z + 2\right)}, z_i\right),$$

where a_i are isolated singularities of the integrand inside of the unit circle. One can rewrite $f(z)$ as

$$f(z) = \frac{z^4 - 2z^2 + 1}{2z^2\left(z + 2\right)\left(z + \frac{1}{2}\right)},$$

to see that it has poles at $z = 0$ and $z = -\frac{1}{2}$ of orders 2 and 1 respectively.

$$\operatorname{Res}\left(f(z), -\frac{1}{2}\right) = \lim_{z\to -\frac{1}{2}} \frac{z^4 - 2z^2 + 1}{2z^2\left(z + 2\right)} = \frac{3}{4}.$$

$$\operatorname{Res}\left(f(z), 0\right) = \lim_{z\to 0} \partial_z \frac{z^4 - 2z^2 + 1}{2z^2 + 5z + 2} = -\frac{5}{4}.$$

Therefore,

$$I = \frac{\pi}{4}.$$

Another class of integrals that can be computed via using Cauchy's theorem is class of rational integrals in real variable over infinite interval. Let $P(z)$ be an entire function, and $Q(z)$ be a polynomial with no real roots. We are interested in evaluation of the integral

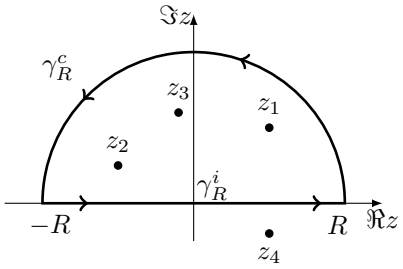
$$I = \int_{-\infty}^{\infty} \frac{P(x)}{Q(x)}\,\mathrm{d}\,x \qquad \text{assuming } \frac{|zP(z)|}{|Q(z)|} \to 0, \quad \text{when} \quad |z| \to \infty, z \in \mathbb{C}_+.$$

In the expression above, $\mathbb{C}_+$ is the upper half complex plane, $\Im z > 0$. By the definition

$$I = \lim_{R\to\infty} I_R, \qquad I_R \coloneqq \int_{-R}^{R} \frac{P(x)}{Q(x)}\,\mathrm{d}\,x,$$

and we would like to consider I_R as a contour integral with contour γ_R given by the interval $(-R, R)$ parametrized with $\gamma_R^i(t) = t$, for $t \in (-R, R)$. Such a contour

is not closed, and therefore the residue theorem is not applicable. However, if one considers contour $\gamma_R = \gamma_R^i \cup \gamma_R^c$ with $\gamma_R^c = \left\{R\,\mathrm{e}^{it} : t \in [0,\pi]\right\}$:



Then

$$I_R = \oint\limits_{\gamma_R} \frac{P(z)}{Q(z)}\,\mathrm{d}\,z - \int\limits_{\gamma_R^c} \frac{P(z)}{Q(z)}\,\mathrm{d}\,z.$$

If R is big enough, then all the singularities (i.e., zeros of $Q(z)$) with positive imaginary part $z_1, z_2, \ldots, z_n$ are trapped inside of γ_R, and therefore the first integral can be calculated by using the residue theorem. For the second one

$$\left| \int\limits_{\gamma_R^c} \frac{P(z)}{Q(z)}\,\mathrm{d}\,z \right| \le 2\pi R \max_{z\in\gamma_R^c} \left|\frac{P(z)}{Q(z)}\right| \to 0, \quad \text{when} R \to \infty.$$

Therefore we obtain

$$I = \lim_{R\to\infty} \int\limits_{-R}^{R} \frac{P(x)}{Q(x)}\,\mathrm{d}\,x = 2\pi i \sum_{z_j} \operatorname{Res}\left(\frac{P(z)}{Q(z)}, z_j\right),$$

where the sum is taken over all zeros of $Q(z)$ in the upper half plane. In some of the cases it is more convenient to close the contour through the bottom half plane $\mathbb{C}_-$. In this case we need to calculate the residues at the poles lying in $\mathbb{C}_-$.

EXAMPLE Let us compute

$$I = \int\limits_{-\infty}^{\infty} \frac{x^2}{\left(x^2+1\right)^2}\,\mathrm{d}\,x.$$

It is obvious that

$$\frac{\left|z^3\right|}{\left|\left(z^2+1\right)^2\right|} \sim \frac{1}{|z|} \to 0, \quad \text{when} \quad |z| \to \infty, z \in \mathbb{C}_+.$$

Therefore,

$$I = 2\pi i \operatorname{Res}\left(\frac{z^2}{\left(z^2+1\right)^2}, i\right),$$

as there is only one singularity of the integrand in an upper half plane. This pole is of the second order and

$$\operatorname{Res}\left(\frac{z^2}{\left(z^2+1\right)^2}, i\right) = \lim_{z\to i} \partial_z \frac{z^2}{(z+i)^2} = -\frac{i}{4}.$$

And the integral is equal to

$$I = \frac{\pi}{2}.$$

2. Integral transformations

2.1. Fourier series. We have seen earlier that any smooth function can be represented as its Taylor series expansion. If the function f is periodic, however, the power series expansion might look less convenient, because the elements of the series do not preserve this property. For periodic functions it is more natural to decompose it into finite or infinite sum of simple periodic functions performing a *Fourier series* expansion.

DEFINITION 2.1 (Fourier series). *Let us consider a function* $f(x) \in L^1[-\pi,\pi] \cap L^2[-\pi,\pi]$*, i.e., such that* $\int_{-\pi}^{\pi} |f(x)|\,\mathrm{d}\,x < +\infty$ *and* $\int_{-\pi}^{\pi} |f(x)|^2\,\mathrm{d}\,x < +\infty$*. Then its Fourier series is defined by*

$$S_f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} \left(a_k \cos(kx) + b_k \sin(kx)\right),$$

where

$$\begin{cases} a_k &= \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\cos(kx)\,\mathrm{d}\,x, \\ b_k &= \frac{1}{\pi}\int_{-\pi}^{\pi} f(x)\sin(kx)\,\mathrm{d}\,x. \end{cases}$$

It is easy to check that if $f(x)$ is a trigonometric polynomial, then its Fourier series is given by itself. Alternatively one can use complex exponents e^{ikx}, $k = 0, \pm1, \pm2, \ldots$ as a basis. Then Fourier series for a function f is given by

$$S_f(x) = \sum_{k=-\infty}^{\infty} c_k\,\mathrm{e}^{ikx},$$

where

$$c_k = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(x)\,\mathrm{e}^{-ikx}\,\mathrm{d}\,x.$$

Fourier series is a way to represent a function as the sum of simple waves. More formally, it decomposes any periodic function or periodic signal into the sum of a (possibly infinite) set of simple oscillating functions, namely sines and cosines (or, equivalently, complex exponentials). Under some additional conditions on smoothness of f it can be shown that its Fourier series converges point-wise, in $L^2[-\pi,\pi]$ norm, uniformly to $f(x)$. One of important properties of Fourier series that it has the same norm as initial function. More precisely

THEOREM 2.1 (Parseval's identity). *Let us consider* $f(x) \in L^1[-\pi,\pi] \cap L^2[-\pi,\pi]$ *with Fourier series*

$$S_f(x) = \frac{a_0}{2} + \sum_{k=1}^{\infty} \left(a_k \cos(kx) + b_k \sin(kx)\right).$$

Then

$$\frac{1}{\pi}\int_{-\pi}^{\pi} |f(x)|^2\,\mathrm{d}\,x = \frac{a_0^2}{2} + \sum_{k=1}^{\infty} \left(a_k^2 + b_k^2\right).$$

EXAMPLE Let us build Fourier series for

$$f(x) = |x|\,, \qquad x \in [-\pi, \pi]\,.$$

All coefficients b_k vanish because of the symmetry

$$b_k = \frac{1}{\pi}\int\limits_{-\pi}^{\pi} |x| \sin(kx)\,\mathrm{d}\,x = 0.$$

For cosine terms we have

$$a_k = \frac{1}{\pi}\int\limits_{-\pi}^{\pi} |x| \cos(kx)\,\mathrm{d}\,x = \frac{2}{\pi}\int\limits_{0}^{\pi} x\cos(kx)\,\mathrm{d}\,x = \begin{cases} \pi, & k = 0 \\ \frac{2}{k^2\pi}\left(\left(-1\right)^k - 1\right), & k > 0. \end{cases}$$

And corresponding Fourier series takes the form

$$S_f(x) = \frac{\pi}{2} - \frac{1}{\pi}\sum_{k=1}^{\infty} \frac{4}{\left(2k+1\right)^2}\cos(2k+1)\,x.$$

Parseval's identity gives

$$\frac{2\pi^3}{3} = \pi\left(\frac{\pi^2}{2} + \frac{16}{\pi^2}\sum_{k=1}^{\infty}\frac{1}{\left(2k+1\right)^4}\right) \Rightarrow \sum_{k=1}^{\infty}\frac{1}{\left(2k+1\right)^4} = \frac{\pi^4}{96}.$$

2.2. Discrete Fourier transform. Let us now introduce the *discrete Fourier transform*.

DEFINITION 2.2. *The discrete Fourier transform maps a sequence of N complex numbers $x_0, x_1, \ldots, x_{N-1}$ into another sequence of complex numbers, $t_0, t_1, \ldots, t_{N-1}$ which is defined by*

$$t_n = \sum_{k=0}^{N-1} x_k\,\mathrm{e}^{-2\pi i k\frac{n}{N}},$$

THEOREM 2.2 (Properties of discrete Fourier transform). *The discrete Fourier transform is an invertible, linear transformation $\mathcal{F}_d : \mathbb{C}^N \to \mathbb{C}^N$ with $\mathbb{C}^N$ denoting the set of N-tuples of complex numbers. The inverse is given by*

$$x_n = \frac{1}{N}\sum_{k=0}^{N-1} t_k\,\mathrm{e}^{2\pi i k\frac{n}{N}}\,.$$

Parseval's identity takes the form

$$\sum_{n=0}^{N-1}\left|x_n\right|^2 = \frac{1}{N}\sum_{n=0}^{N-1}\left|t_n\right|^2.$$

2.3. Fourier transform. Continuous analogue of the Fourier series and the discrete Fourier transform is Fourier transform.

DEFINITION 2.3 (Fourier transform). *Let $f \in L^1(\mathbb{R})$ be an absolutely integrable function on $\mathbb{R}$. Then its Fourier transform $\hat{f}(t)$ is defined by*

$$\hat{f}(t) \equiv \mathcal{F}[f](t) \coloneqq \int\limits_{-\infty}^{\infty} \mathrm{e}^{ixt}\,f(x)\,\mathrm{d}\,x.$$

The condition $f \in L^1(\mathbb{R})$ yields that $f(x)$ must be defined from $-\infty$ to ∞ and in particular it is necessary that $f(x) \to 0$ for $x \to \pm\infty$. Observe that in the following we will denote, for the sake of brevity, $\hat{f}(t)$ as the Fourier transform of f.

THEOREM 2.3 (Parseval's identity). *Let $f \in L^1(\mathbb{R}) \cap L^2(\mathbb{R})$ be an absolutely integrable with its square function on $\mathbb{R}$. Then $\hat{f}(t) \in L^2(\mathbb{R})$ and*

$$2\pi \int_{-\infty}^{\infty} |f(x)|^2 \,\mathrm{d}\, x = \int_{-\infty}^{\infty} |\hat{f}(t)|^2 \,\mathrm{d}\, t.$$

THEOREM 2.4. *The Fourier transform is a linear map $\mathcal{F} : L^1(\mathbb{R}) \to L^\infty(\mathbb{R})$. For functions $f \in L^1(\mathbb{R})$ with $\hat{f} \in L^1(\mathbb{R})$ one can define inverse Fourier transform by*

$$\mathcal{F}^{-1}[\hat{f}](x) \coloneqq \frac{1}{2\pi} \int_{-\infty}^{\infty} \mathrm{e}^{-ixt}\, \hat{f}(t) \,\mathrm{d}\, t.$$

If additionally f is continuous, then

$$f(x) = \mathcal{F}^{-1}[\hat{f}](x), \quad \forall x \in \mathbb{R}.$$

THEOREM 2.5 (Properties of Fourier transform). *Let f, g be smooth, absolutely integrable with all their derivatives functions defined on $\mathbb{R}$. Then*

(1) $\mathcal{F}\left[f\left(x - x_0\right)\right](t) = \mathrm{e}^{itx_0}\, \hat{f}(t)$.
(2) $\mathcal{F}\left[f\left(ax\right)\right](t) = \frac{1}{a} \hat{f}\left(t/a\right)$.
(3) $\mathcal{F}\left[f^{(n)}\right](t) = (-it)^n\, \hat{f}(t)$.
(4) $\mathcal{F}\left[f * g\right](t) = \hat{f}(t)\hat{g}(t)$, *where $f * g$ is a convolution defined by*

$$\left(f * g\right)(x) = \int_{-\infty}^{\infty} f\left(x - y\right) g(y) \,\mathrm{d}\, y.$$

(5) $\mathcal{F}\left[1\right](t) = 2\pi\delta(t)$, $\mathcal{F}^{-1}\left[\delta\right](t) = \frac{1}{2\pi}$, *where δ is the Dirac delta function.*

☞ *Link to white noise* A white noise $X(t)$ is defined as a stochastic function of time with the properties:

$$\langle X \rangle = 0 \qquad \langle X(t)X(t') \rangle = C\delta(t - t')$$

i.e. the correlation in time is given by a δ-function (i.e. the values of $X(t)$ are uncorrelated for $t \neq t'$). The FT of this correlation function, called *power spectrum* (i.e. the correlation in the space of frequencies) is a constant by Theorem 2.5, which implies that all the frequencies contribute to it with the same weight (as it happens for white light).

EXAMPLE For $a \in \mathbb{R}$, let

$$f_a(x) \equiv \theta(x - a) = \begin{cases} 0, & x \leq a \\ 1, & x > a. \end{cases}$$

Let us compute $f_a * f_b$ for $a, b \in \mathbb{R}$. Using the definition

$$(f_a * f_b)(x) = \int_{-\infty}^{\infty} f_a(x-y)\, f_b(y)\, \mathrm{d}\, y = \begin{cases} \int_b^{x-a} \mathrm{d}\, y = x-a-b & x > b+a \\ 0, & x < b+a. \end{cases}$$

Therefore,

$$(f_a * f_b)(x) = (x-a-b)\, f_{a+b}(x).$$

EXAMPLE For $a \in \mathbb{R}_+$, let

$$g_a(x) = \begin{cases} 0, & x \le 0 \\ \mathrm{e}^{-ax}, & x > 0. \end{cases}$$

Let us compute $g_a * g_b$ for $a, b \in \mathbb{R}$. Using the definition

$$(g_a * g_b)(x) = \int_{-\infty}^{\infty} g_a(x-y)\, g_b(y)\, \mathrm{d}\, y = \int_0^{\infty} \mathrm{e}^{-a(x-y)}\, \mathbb{I}(x-y>0)\, \mathrm{e}^{-by}\, \mathrm{d}\, y$$

$$= \begin{cases} \frac{\mathrm{e}^{-bx} - \mathrm{e}^{-ax}}{a-b} & x > 0, a \neq b \\ x\, \mathrm{e}^{-ax} & x > 0, a = b \\ 0, & x \le 0. \end{cases}$$

Fourier transform of g_a is given by

$$\mathcal{F}[g_a](t) = \int_{-\infty}^{\infty} \mathrm{e}^{ixt-ax}\, \theta(x)\, \mathrm{d}\, x = \int_0^{\infty} \mathrm{e}^{-(a-it)x}\, \mathrm{d}\, x = \frac{1}{a-it}.$$

Using properties of Fourier transform we obtain

$$\mathcal{F}[g_a * g_b](t) = \frac{1}{a-it}\frac{1}{b-it} = \frac{1}{b-a}\left(\frac{1}{a-it} - \frac{1}{b-it}\right)$$

$$= \frac{1}{b-a}\left(\mathcal{F}[g_a](t) - \mathcal{F}[g_b](t)\right) = \mathcal{F}\left[\frac{g_a - g_b}{b-a}\right](t), \quad a \neq b.$$

2.3.1. *Calculation of Fourier transforms.* The residue theorem can be used to evaluate also integrals of the from

$$\hat{f}(t) = \int_{-\infty}^{\infty} \mathrm{e}^{ixt}\, f(x)\, \mathrm{d}\, x.$$

We start with the definition

$$\int_{-\infty}^{\infty} \mathrm{e}^{itx}\, f(x)\, \mathrm{d}\, x = \lim_{R\to\infty} \int_{-R}^{R} \mathrm{e}^{itx}\, f(x)\, \mathrm{d}\, x.$$

Then we consider a complex integral along the contour γ_R as in the figure in Section 1.2 in such a way that

$$\oint_{\gamma_R} \mathrm{e}^{itz}\, f(z)\, \mathrm{d}\, z = \int_{-R}^{R} \mathrm{e}^{itx}\, f(x)\, \mathrm{d}\, x + \int_{\gamma_R^c} \mathrm{e}^{itz}\, f(z)\, \mathrm{d}\, z = 2\pi\mathrm{i} \sum_{a_j} \mathrm{Res}\left(\mathrm{e}^{itz} f, a_j\right),$$

where a_j are the singularities of $f(z)$ in the upper half plane. We can evaluate this integral by residue theorem, as shown by the last equality. For the semicircular part we can use

LEMMA 2.6 (Jordan's lemma). *Consider a complex-valued, continuous function h, defined on a semicircular contour $\gamma_R^c = \left\{R\,\mathrm{e}^{it} : t \in [0,\pi]\right\}$ of positive radius R lying in the upper half-plane, centred at the origin. If the function h is of the form*

$$h(z) = \mathrm{e}^{iaz}\, g(z), \qquad z \in \gamma_R^c,$$

with a positive parameter a, then

$$\left| \int_{\gamma_R^c} h(z)\,\mathrm{d}\,z \right| \leq \frac{\pi}{a} \max_{t\in[0,\pi]} \left| g\left(R\,\mathrm{e}^{i\theta}\right)\right|.$$

An analogous statement for a semicircular contour in the lower half-plane holds when $a < 0$.

If function $f(z)$ decays fast in upper half plane, then in the limit of $R \to \infty$ we can use the lemma to show

$$\lim_{R\to\infty} \int_{\gamma_R^c} \mathrm{e}^{itz}\, f(z) = 0, \quad t > 0.$$

provided that $\lim_{|z|\to\infty} f(z) = 0$. As a consequence, the integral along γ_R^c vanishes and the residue formula actually allows one to evaluate $\int_{-\infty}^{\infty} \mathrm{e}^{itx}\, f(x)\,\mathrm{d}\,x$.

EXAMPLE [From the exam CS04, Problem 3.5 with $\gamma = 0$] Consider a forced one-dimensional harmonic oscillator with mass m, natural frequency ω_0

$$\ddot{x}(t) + \omega_0^2 x(t) = \frac{f(t)}{m}.$$

Assume the displacement $x(t)$ from the equilibrium position $x(t) \equiv 0$ in presence of the force $f(t)$ is given by convolution of the force and response function, i.e.

$$x(t) = (R * f)(t) = \int_{-\infty}^{\infty} R(t-s)\, f(s)\,\mathrm{d}\,s,$$

where $R(t)$ is the response function. Define the dynamical susceptibility $\chi(\omega)$ as the Fourier transform of the response function

$$\chi(\omega) = \mathcal{F}[R](\omega) = \int_{-\infty}^{\infty} R(t)\,\mathrm{e}^{i\omega t}\,\mathrm{d}\,t.$$

Then, using properties of the Fourier transform, we can get

$$\mathcal{F}[x](\omega) = \mathcal{F}[R](\omega)\mathcal{F}[f](\omega) = \chi(\omega)\hat{f}(\omega).$$

For the second derivative we have

$$\mathcal{F}[\ddot{x}](\omega) = -\omega^2 \mathcal{F}[x](\omega) = -\omega^2 \chi(\omega)\hat{f}(\omega).$$

taking Fourier transform of initial equation we obtain

$$\left(\omega_0^2 - \omega^2\right)\chi(\omega)\hat{f}(\omega) = \frac{1}{m}\hat{f}(\omega),$$

and we obtain

$$\chi(\omega) = \frac{1}{m\,(\omega_0^2 - \omega^2)}.$$

EXAMPLE [From exam CS04, Problem 3.5 with $\gamma > 0$] Consider a forced one-dimensional harmonic oscillator with mass m, natural frequency ω_0 and damping constant $\gamma > 0$.

$$\ddot{x}(t) + \frac{\gamma}{m}\dot{x}(t) + \omega_0^2 x(t) = \frac{f(t)}{m}.$$

In the same notation of the previous example, and repeating above calculation one can get

$$\chi(\omega) = \frac{1}{m\,(\omega_0^2 - \omega^2 - i\gamma\omega)}.$$

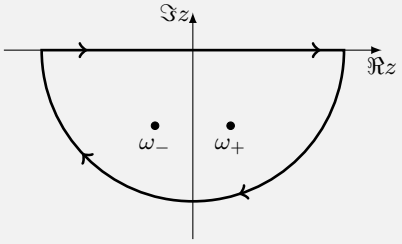
We now want to calculate the response function by using the inverse Fourier transform,

$$R(t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} \mathrm{e}^{-i\omega t}\,\chi(\omega)\,\mathrm{d}\,\omega. \tag{11}$$

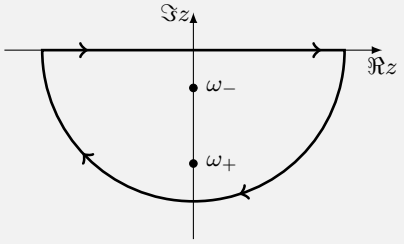
The function $\chi(\omega)$ has two poles at

$$\omega_\pm = \frac{-i\gamma \pm \sqrt{4\omega_0^2 - \gamma^2}}{2}.$$

If $\omega_0 > \frac{\gamma}{2}$, then $\Im\omega_\pm = \frac{-\gamma}{2}, \Re\omega_\pm = \pm\sqrt{\omega_0^2 - \frac{\gamma^2}{4}}$ and $\omega_\pm$ are complex numbers lying in the bottom half plane. If $\omega_0 < \frac{\gamma}{2}$, then $\Re\omega_\pm = 0, \Im\omega_\pm = -\frac{\gamma}{2} \pm \sqrt{\frac{\gamma^2}{4} - \omega_0^2}$ and $\omega_\pm$ are pure imaginary numbers lying in the bottom half plane.



$\omega_0 > \frac{\gamma}{2}$



$\omega_0 < \frac{\gamma}{2}$

For $t > 0$ we close the contour as in the pictures above. The integral along the semicircle goes to 0, as $\chi(\omega) \sim \omega^{-2}$, when $\omega \to \infty$. By the residue theorem

$$\begin{aligned} R(t) = i\,(\mathrm{Res}_{\omega_1} + \mathrm{Res}_{\omega_2})\,\mathrm{e}^{-i\omega t}\,\chi(\omega) &= -\frac{i}{m}\left(\frac{\mathrm{e}^{-i\omega_1 t}}{\omega_2 - \omega_1} + \frac{\mathrm{e}^{-i\omega_2 t}}{\omega_1 - \omega_2}\right) \\ &= \frac{i}{m}\frac{\mathrm{e}^{-i\omega_1 t} - \mathrm{e}^{-i\omega_2 t}}{\omega_1 - \omega_2} = \mathrm{e}^{-\gamma t/2}\,\frac{\sin\left(t\sqrt{\omega_0^2 - \gamma^2/4}\right)}{m\sqrt{\omega_0^2 - \gamma^2/4}}. \end{aligned}$$

For $t < 0$ we close the contour through the upper half plane, where no poles are present and therefore $R(t) = 0$. Finally,

$$R(t) = \mathrm{e}^{-\gamma t/2}\,\frac{\sin\left(t\sqrt{\omega_0^2 - \gamma^2/4}\right)}{m\sqrt{\omega_0^2 - \gamma^2/4}}\theta(t).$$

EXAMPLE [From CS04, Exercise 3.3] *Question:* Equilibrium correlations normally decay with a characteristic decay time τ_C, as $C(\tau) = \mathrm{e}^{-\frac{\tau}{\tau_C}}$. Show that the power spectrum (i.e. the Fourier transform of the correlation function) is

$$S(\omega) = \frac{2\tau_C}{\omega^2\tau_C^2 + 1}.$$

Solution: Instead of calculating Fourier transform of correlation function

$$\mathcal{F}[C](\omega) = \int_{-\infty}^{\infty} \mathrm{e}^{i\omega\tau - \frac{\tau}{\tau_C}}\,\mathrm{d}\,\tau,$$

we will show that inverse Fourier transform of $S(\omega)$, given by

$$\mathcal{F}^{-1}[S](\tau) = \frac{\tau_C}{\pi}\int_{-\infty}^{\infty} \frac{\mathrm{e}^{-i\omega\tau}}{\omega^2\tau_C^2 + 1}\,\mathrm{d}\,\omega$$

is equal to $C(\tau)$. For the last integral we use Jordan's lemma 2.6 to change the contour to the bottom semicircular for $\tau > 0$ and upper for $\tau < 0$. Then the integral can be calculated by the residue theorem:

$$\begin{cases} \mathcal{F}^{-1}[S](\tau) = -2i\tau_C \mathrm{Res}\left(\frac{\mathrm{e}^{-iz\tau}}{z^2\tau_C^2+1}, -\frac{i}{\tau_C}\right) = -2i\tau_C \frac{1}{-2i\tau_C}\,\mathrm{e}^{-\frac{\tau}{\tau_C}} = C(\tau), & \tau > 0; \\ \mathcal{F}^{-1}[S](\tau) = 2i\tau_C \mathrm{Res}\left(\frac{\mathrm{e}^{-iz\tau}}{z^2\tau_C^2+1}, \frac{i}{\tau_C}\right) = 2i\tau_C \frac{1}{2i\tau_C}\,\mathrm{e}^{-\frac{\tau}{\tau_C}} = C(\tau), & \tau < 0. \end{cases}$$

where in the first case we put minus sign in front of the residues because the contour is clockwise oriented. For $\tau = 0$ one can check identity directly

$$\mathcal{F}^{-1}[S](0) = \frac{\tau_C}{\pi}\int_{-\infty}^{\infty} \frac{1}{\omega^2\tau_C^2 + 1}\,\mathrm{d}\,\omega = 1.$$

2.3.2. *Multidimensional Fourier transform.* One can also define Fourier transform for multivariate functions.

DEFINITION 2.4 (Fourier transform). *Let $f \in L^1(\mathbb{R}^d)$ be an absolutely integrable function on $\mathbb{R}^d$, i.e., $\int_{\mathbb{R}^d} |f(\boldsymbol{x})|\,\mathrm{d}\,\boldsymbol{x} < \infty$. Then its Fourier transform is defined by*

$$\mathcal{F}[f](\boldsymbol{t}) = \int_{\mathbb{R}^d} \mathrm{e}^{i\langle \boldsymbol{t}, \boldsymbol{x}\rangle}\, f(\boldsymbol{x})\,\mathrm{d}\,\boldsymbol{x}.$$

THEOREM 2.7 (Parseval's identity). *Let $f \in L^1(\mathbb{R}^d) \cap L^2(\mathbb{R}^d)$ be an absolutely integrable with its square function on $\mathbb{R}^d$. Then $\mathcal{F}[f] \in L^2(\mathbb{R}^d)$ and*

$$(2\pi)^d \int_{\mathbb{R}^d} |f(\boldsymbol{x})|^2\,\mathrm{d}\,\boldsymbol{x} = \int_{\mathbb{R}^d} |\mathcal{F}[f](\boldsymbol{t})|^2\,\mathrm{d}\,\boldsymbol{t}.$$

THEOREM 2.8. *The Fourier transform is a linear map $\mathcal{F}\colon L^1(\mathbb{R}^d) \to L^\infty(\mathbb{R}^d)$. For functions $f \in L^1(\mathbb{R}^d)$ with absolutely integrable Fourier transform $\hat{f} := \mathcal{F}[f] \in L^1(\mathbb{R}^d)$ one can define inverse Fourier transform by*

$$\mathcal{F}^{-1}[\hat{f}](\boldsymbol{x}) = \frac{1}{(2\pi)^d}\int_{\mathbb{R}^d} \mathrm{e}^{-i\langle \boldsymbol{t}, \boldsymbol{x}\rangle}\, \hat{f}(\boldsymbol{t})\,\mathrm{d}\,\boldsymbol{t}.$$

If additionally f is continuous, then

$$f(\boldsymbol{x}) = \mathcal{F}^{-1}[\hat{f}](\boldsymbol{x}), \quad \forall \boldsymbol{x} \in \mathbb{R}.$$

EXAMPLE Let $f(x,y) = \exp\left\{-x^2/2 + \lambda xy - y^2/2\right\}$ for $|\lambda| < 1$. The corresponding Fourier transform is given by

$$\mathcal{F}[f](\boldsymbol{t}) = \int\limits_{\mathbb{R}^2} \mathrm{e}^{-\frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle + i\langle \boldsymbol{t}, \boldsymbol{x}\rangle}\, \mathrm{d}\,\boldsymbol{x} = \frac{2\pi}{\sqrt{\det \boldsymbol{A}}}\, \mathrm{e}^{-\left\langle \boldsymbol{t}, \boldsymbol{A}^{-1}\boldsymbol{t}\right\rangle},$$

where $\boldsymbol{A} = \left(\begin{smallmatrix} 1 & -\lambda \\ -\lambda & 1 \end{smallmatrix}\right)$ and we used the value of Gaussian integral obtained before. One can easily find $\boldsymbol{A}^{-1} = \frac{1}{1-\lambda^2}\left(\begin{smallmatrix} 1 & \lambda \\ \lambda & 1 \end{smallmatrix}\right)$ and therefore

$$\mathcal{F}[f](\boldsymbol{t}) = \frac{2\pi}{1-\lambda^2}\, \mathrm{e}^{-\frac{t_1^2}{1-\lambda^2} - 2\frac{\lambda t_1 t_2}{1-\lambda^2} - \frac{t_2^2}{1-\lambda^2}}.$$

2.4. Laplace transform. The Laplace transform is an integral transform defined as

DEFINITION 2.5. *Let $f : \mathbb{R}_+ \to \mathbb{C}$ be a complex valued function defined on a positive semiaxis. Its Laplace transform is a function defined in complex plane by*

$$\mathcal{L}[f](s) = \int\limits_0^\infty \mathrm{e}^{-sx}\, f(x)\, \mathrm{d}\, x.$$

In probability theory Laplace transform of a probability distribution for real positive random variable is its moment generating function. The following theorem holds.

THEOREM 2.9. *Let $f \in L^\infty(\mathbb{R})$ be an absolutely integrable complex valued function on $\mathbb{R}_+$. Then its Laplace transform $F(s)$ is an analytic function in the region of its convergence and inverse Laplace transform is given by Mellin's inverse formula:*

$$\mathcal{L}^{-1}[F](x) = \frac{1}{2\pi i} \int\limits_{\gamma - i\infty}^{\gamma + i\infty} \mathrm{e}^{st}\, F(s)\, \mathrm{d}\, s,$$

where γ is a real number so that the contour path of integration is in the region of convergence of $F(s)$.

THEOREM 2.10. *Let $f \in L^\infty(\mathbb{R})$ be absolutely integrable with all its derivatives on $\mathbb{R}$ and let $F(s)$ be its Laplace transform. We introduce*

$$\mathcal{I}[f](t) = \int\limits_0^t f(s)\, \mathrm{d}\, s,$$

being anti-derivative of $f(s)$. Then

(1) $\mathcal{L}[f(ax)](s) = \frac{1}{a} F\left(\frac{s}{a}\right)$.
(2) $\mathcal{L}[f'(x)](s) = sF(s) - f(0)$.
(3) $\mathcal{L}[f''(x)](s) = s^2 F(s) - sf(0) - f'(0)$.
(4) $\mathcal{L}\left[f^{(n)}(x)\right](s) = s^n F(s) - \sum_{j=0}^{n-1} s^j f^{(n-j-1)}(0)$.
(5) $\mathcal{L}[\mathcal{I}[f](x)](s) = \frac{F(s)}{s}$.
(6) $\mathcal{L}[\delta(x - x_0)](s) = \mathrm{e}^{-sx_0} \begin{cases} 1 & \text{if} \quad x_0 > 0, \\ 0 & \text{if} \quad x_0 \le 0. \end{cases}$

EXAMPLE [Magnetization distribution for non-interacting spins] Consider N spins variables $\sigma_i \in \{-1, 1\}$, with $i = 1, \dots, N$ and define the total magnetization $M = \sum_i \sigma_i$. In the absence of external magnetic field ($h = 0$) and spin-spin interactions, σ_i's are i.i.d. variables with distribution

$$p(\sigma) = \frac{1}{2}\delta_{\sigma,1} + \frac{1}{2}\delta_{\sigma,-1}.$$

Then, the number of configurations compatible with some magnetisation M is given by the partition function

$$Z(M) = \sum_{\boldsymbol{\sigma}} \prod_{i=1}^{N} p(\sigma_i)\, \delta\left(M - \sum_i \sigma_i\right),$$

To calculate the partition function the easiest way is to compute its Laplace transform, given the factorising property of the Laplace transform

$$\begin{aligned} \hat{Z}(\alpha) = & \int_0^\infty \mathrm{e}^{-\alpha M} Z(M)\, \mathrm{d}\, M = \sum_{\boldsymbol{\sigma}} \prod_{i=1}^{N} p(\sigma_i) \int_0^\infty \mathrm{e}^{-\alpha M}\, \delta\left(M - \sum_i \sigma_i\right) \mathrm{d}\, M \\ = & \sum_{\boldsymbol{\sigma}} \prod_{i=1}^{N} p(\sigma_i)\, \mathrm{e}^{-\alpha \sigma_i} = (\cosh \alpha)^N. \end{aligned}$$

$Z(M)$ can then be found by using the inversion formula

$$Z(M) = \int_{c-i\infty}^{c+i\infty} \mathrm{e}^{\alpha M}\, \hat{Z}(\alpha)\, \mathrm{d}\, \alpha = \int_{c-i\infty}^{c+i\infty} \mathrm{e}^{\alpha M + N \log\cosh \alpha}\, \mathrm{d}\, \alpha,$$

where c must be chosen to the right of any singularity. For large N, one can evaluate the integral using the saddle-point (or Laplace) method, which consists in approximating the integral with its largest integrand, found by locating the maximum of the exponent. We obtain, with $m = M/N$,

$$Z(M) \sim \mathrm{e}^{N s(m)},$$

where

$$\begin{aligned} s(m) = & \sup_\alpha [\alpha m + \log\cosh \alpha] \\ = & -m\, \mathrm{atanh}\, m + \ln 2 \cosh(\mathrm{atanh}\, m) \\ = & -\frac{1+m}{2} \ln\left(\frac{1+m}{2}\right) - \frac{1-m}{2} \ln\left(\frac{1-m}{2}\right), \end{aligned}$$

which is the constrained entropy, or log-density of states exhibiting magnetization m. The interpretation is clear: to achieve the total magnetization m, each spin will have to take values ± 1 with probabilities $(1 \pm m)/2$. Hence $s(m)$ is the Shannon entropy of a system with these probabilities.

2.4.1. *Tail behaviour extraction from Laplace transform.* Suppose that $f(t)$ has some tail for large t that is expressed by a power law, i.e.

$$f(t) \sim t^{-\mu} \qquad t \gg 1,$$

with $\mu < 1$, in such a way that $\int_0^\infty t^{-\mu} dt$ diverges. $\mathcal{L}[f](s)$ depends on the whole $f(t)$ but one can extract some information on its small s asymptotics from the tail behavior of f. Indeed, for small s,

$$\mathcal{L}[f](s) \sim \int_0^\infty t^{-\mu}\, \mathrm{e}^{-st}\, \mathrm{d}\, t = s^{\mu-1}\Gamma(1-\mu) \qquad \mu < 1,$$

where we have set $x = st$ and we have introduced the Γ function

$$\Gamma(n) = \int_0^\infty x^{n-1}\,\mathrm{e}^{-x}\,\mathrm{d}\,x.$$

Therefore, if a priori we know that $f(t)$ has a power law decay at infinity, then we can find exact asymptotics of it just by analysing its Laplace transform asymptotics around zero.

Exercises

(1) Show that $f(z) = z^n$ is an entire function and prove its derivative is given by $f'(z) = nz^{n-1}$.
(2) Calculate the integral

$$\int_\gamma \frac{\sin\frac{1}{z}}{z^2\left(z^2-4z+5\right)}\,\mathrm{d}\,z,$$

where γ is
   (a) Circle of radius 1 around the origin.
   (b) Circle of radius $3/2$ around $z = 2$.

(3) Calculate the integral

$$\int_{-\infty}^{\infty} \frac{\sin x}{x}\,\mathrm{d}\,x,$$

via considering corresponding complex integral and closing the contour.
(4) Compute the Fourier transform for $f(x) = 1/x$.
(5) Calculate Fourier transform $\mathcal{F}[f](t)$ for
   (a) $f(x) = \begin{cases} \cos 3x, & x \in [-\pi, \pi]\,, \\ 0, & \text{otherwise.} \end{cases}$
   (b) $f(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\,\mathrm{e}^{-\frac{(x-\mu)^2}{2\sigma^2}}$.
   (c) $f(x) = \begin{cases} x+1, & x \in [-1, 0]\,, \\ 1-x, & x \in (0, 1]\,, \\ 0, & \text{otherwise.} \end{cases}$
   (d) $f(x) = \begin{cases} 0, & x \in (-\infty, 0]\,, \\ \mathrm{e}^{-t}, & t \in [0, \infty)\,. \end{cases}$
   (e) $f(x) = \left(x^2-1\right)\mathrm{e}^{-\frac{x^2}{2}}$.
(6) Calculate the partition function of the system described by Hamiltonian

$$H(\boldsymbol{\sigma}) = -\frac{J}{2N}\sum_{ij}\sigma_i\sigma_j,$$

via using Fourier representation of delta function.

LECTURE 4

Probability

1. Random variables

We start with formal definition of probability space and probability distribution

DEFINITION 1.1. *Let Ω be a set, called sample space and let $\mathcal{F}$ be a σ-algebra of subsets of Ω, called event space, i.e., an algebra of subset of Ω satisfying the following*

1. *$\emptyset, \Omega \in \mathcal{F}$;*
2. *if $A \in \mathcal{F}$, then $A^c \in \mathcal{F}$, i.e. $\mathcal{F}$ is closed under taking complement;*
3. *if $A_i \in \mathcal{F}$ for any $i = 1, 2, \dots$ then $\bigcup_i A_i \in \mathcal{F}$, i.e. $\mathcal{F}$ is closed under union.*

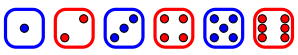
Let $\mathbb{P} \colon \mathcal{F} \to \mathbb{R}$ be a function on $\mathcal{F}$, called probability distribution. We then say that triple $(\Omega, \mathcal{F}, \mathbb{P})$ forms a probability space if the following holds

1. *$\mathbb{P}(\emptyset) = 0$ and $\mathbb{P}(\Omega) = 1$;*
2. *$\mathbb{P}$ is non-negative function;*
3. *for any disjoint $A, B \in \mathcal{F}$, $\mathbb{P}[A \cup B] = \mathbb{P}[A] + \mathbb{P}[B]$.*

DEFINITION 1.2. *Let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space. We call random variable. $X \colon \Omega \to \mathbb{R}$ any measurable function with respect to $\mathcal{F}$.*

To give an example of this formal definition, suppose that we perform an experiment and, every time we repeat it, this has an outcome ω. The outcome can be described by *random variable* $X(\omega)$, related for example to some measurable observable. Its value cannot be specified a priori but we can assign to it a probability $\mathbb{P}[\omega]$ for its occurrence. Each possible outcome ω is a "sample" in the language of probability theory and it belongs to the *sample space* Ω, i.e., the set of all possible outcomes. An *event* is a set of outcomes. The σ-algebra $\mathcal{F}$ is just the family of potentially observable events and it is sometimes called *event space*.

For example, the space Ω of all outcomes of a dice rolling is



The event *even number* corresponds to a subset of tree outcomes.

In the definition above, the function $\mathbb{P}$ is just given. A possible interpretation of it is the following. If we repeat the experiment N times and $n(\omega)$ is the number of times a certain outcome ω appears, $\frac{n(\omega)}{N}$ is the *frequency* of ω. The probability $\mathbb{P}[\omega]$ can be interpreted as the limit of the frequency for increasing N, i.e.

$$\mathbb{P}[\omega] \coloneqq \lim_{N \to \infty} \frac{n(\omega)}{N}.$$

Now we are going to discuss three fundamentally different cases of Ω:

(1) Let Ω contains just one element. This means that there is only one possible outcome ω of the experiment. As a result, any random variable takes only one possible value $X(\omega)$ with probability $\mathbb{P}[\omega] = \mathbb{P}[\Omega] = 1$. This random variable is then *deterministic*.
(2) If $\Omega = \{\omega_i\}_i$ is a countable set, then $\mathcal{F}$ is a collection of *all* possible subsets of Ω, i.e. $\mathcal{F} = 2^{|\Omega|}$, which is possibly infinite. Random variables in this case are said to be *discrete* random variables and can take only countably many values. With any outcome we can assign corresponding probability $\mathbb{P}[\omega_i] \equiv p_i$. As a simple consequence of the definition we can get
$$\sum_{\omega\in\Omega} \mathbb{P}[\omega] = 1.$$
(3) Finally, if Ω contains uncountably infinite number of possible outcomes we say that we have *continuous* probability space. Corresponding random variables are called continuous, and in this case there is no sense (in general) to talk about the probability $\mathbb{P}[\omega]$. Instead of this we discuss probability that an outcome falls into some set $A \in \mathcal{F}$. The normalisation condition in this case is written as
$$\int_{\Omega} \mathbb{P}[\mathrm{d}\,\omega] = 1.$$

1.1. Probability distributions, moments and cumulants.

Definition 1.3. *The cumulative distribution function of a real-valued random variable X is the function defined on a real line and given by*
$$\Phi_X(x) = \mathbb{P}[X \le x] \coloneqq \mathbb{P}[\omega \in \Omega\colon X(\omega) < x],$$
where the right-hand side represents the probability that the random variable X takes on a value less than or equal to x.

Some basic and general properties of Φ_X follow directly from the definition.

Proposition 1.1. *Let X be a random variable defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Then Φ_X is non-decreasing and right-continuous function on $\mathbb{R}$ and moreover*
$$\lim_{x\to-\infty} \Phi_\phi(x) = 0, \qquad \lim_{x\to\infty} \Phi_\phi(x) = 1.$$

Observe that if X is a purely discrete random variable, then Φ_X will be discontinuous at the points x_i and constant in between. If Φ_X of a real valued random variable X is continuous, then X is a continuous random variable.

Definition 1.4. *Let X be a discrete real random variable with sample space $\Omega = \{\omega_i\}_i$. Then the corresponding probability distribution function $P_X\colon \mathbb{R} \to [0, 1]$ is defined by*
$$P_X(x) = \mathbb{P}[X = x] = \mathbb{P}[\omega \in \Omega\colon X(\omega) = x].$$
Denoting by $x_i = X(\omega_i)$ and by $p_i \coloneqq \mathbb{P}[X = x_i]$, the corresponding cumulative Φ_X is then
$$\Phi_\phi(x) = \sum_{x_i\le x} p_i.$$

DEFINITION 1.5. *Let X be a continuous random variable with absolutely continuous Φ_X. Then there exists function $\rho_X : \mathbb{R} \to \mathbb{R}_+$, called probability density function of X, such that for any real $a < b$*

$$\int_a^b \rho_X(x)\,\mathrm{d}\,x = \Phi_X(b) - \Phi_X(a) = \mathbb{P}[X \in (a,b]].$$

Roughly speaking

$$\rho_X(x) = \partial_x \Phi_\phi(x),$$

and using properties of cumulative Φ_X we can write

$$\Phi_\phi(x) = \int_{-\infty}^{x} \rho_X(x)\,\mathrm{d}\,x.$$

DEFINITION 1.6. *Let X be a real valued random variable defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. We call*

$$\begin{cases} \mathbb{E}[X] = \sum_i x_i P_X(x_i), \text{ (discrete probability space)} \\ \mathbb{E}[X] = \int_{\mathbb{R}} x\rho(x)\,\mathrm{d}\,x, \text{ (continuous probability space)} \end{cases}$$

by its expectation or average. Similarly, for any function $f\colon \mathbb{R} \to \mathbb{R}$ we have that $\mathbb{E}[f(X)] = \sum_i x_i P_X(x_i)$ for a discrete variable X and $\mathbb{E}[f(X)] = \int f(x)\rho(x)\,\mathrm{d}\,x$ for a continuous variable X.

Usually, if there is no ambiguous in the sense of probability measure, we will write $\langle X \rangle$ to denote expectation $\mathbb{E}[X]$. Expectation of random variable gives a typical value of it, however it doesn't mean that the RV is close to this value. The quality of approximation is defined by the square root of variance:

DEFINITION 1.7. *Let X be a random variable defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. Then*

$$\mathrm{Var}[X] = \left\langle (X - \langle X \rangle)^2 \right\rangle = \left\langle X^2 \right\rangle - \langle X \rangle^2,$$

is called variance of RV X.

DEFINITION 1.8. *Let X be a random variable defined on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$. We call average of its nth power by its nth moment, i.e.*

$$\mu_n = \begin{cases} \sum_i x_i^n P_X(x_i), \text{ (discrete probability space)} \\ \int_{\mathbb{R}} x^n \rho(x)\,\mathrm{d}\,x, \text{ (continuous probability space).} \end{cases}$$

DEFINITION 1.9. *The moment generating function for a RV X is defined as*

$$M_X(t) = \left\langle \mathrm{e}^{tX} \right\rangle.$$

The moments of X can be obtained by derivation, i.e.

$$\langle X^n \rangle = \frac{\mathrm{d}^n}{\mathrm{d}\,t^n} M_X(t) \bigg|_{t=0}.$$

The last statement follows from the Taylor series expansion of the exponent. Let us write (without rigorous explanation)

$$M_X(t) = \left\langle \sum_{k=0}^{\infty} \frac{t^k X^k}{k!} \right\rangle = \sum_{k=0}^{\infty} \frac{t^k \left\langle X^k \right\rangle}{k!} = \sum_{k=0}^{\infty} \frac{t^k \mu_k}{k!}.$$

DEFINITION 1.10. *The characteristic function for a RV X is defined as*

$$\chi_X(t) = \left\langle \mathrm{e}^{itX} \right\rangle .$$

The moments of X can be obtained by derivation, i.e.

$$\langle X^n \rangle = i^{-n} \frac{\mathrm{d}^n}{\mathrm{d}\, t^n} \chi_X(t) \Big|_{t=0} .$$

PROPOSITION 1.2. *The characteristic function χ_X for a RV X satisfies*

$$\chi_X(0) = 1, \quad |\chi_X(t)| \leq 1, \quad t \in \mathbb{R}.$$

The variance of a RV X is an example of an important set of quantities that can be thought as an alternative to the moments, called *cumulants*.

DEFINITION 1.11. *The cumulant generating function for a RV X is defined as*

$$K_X(t) = \ln \left\langle \mathrm{e}^{tX} \right\rangle .$$

The cumulants of X are given by

$$\langle\!\langle X^n \rangle\!\rangle \coloneqq \frac{\mathrm{d}^n}{\mathrm{d}\, t^n} K_X(t) \Big|_{t=0} .$$

By definition, $\langle\!\langle X \rangle\!\rangle = \mathbb{E}[X]$ and $\langle\!\langle X^2 \rangle\!\rangle = \mathrm{Var}[X]$.

EXAMPLE Consider throwing two dices at the same time. What is the average sum we will get? What is the average deviation from the average sum? We deal with discrete random variable in this case. There are 36 possible outcomes $\Omega = \{(a,b)\}_{a,b=1}^{6}$ with equal probabilities $\frac{1}{36}$ (we assume that we have fair dices). Let X_A be the random variable reporting the number associated to the outcome of the rolling of the dice A, taking values in $\{a\}_{a=1}^{6}$, and similarly X_B the outcome of the dice B, taking values in the same set $\{b\}_{b=1}^{6}$. Our random variable is $X = X_A + X_B$ and therefore

$$\langle X \rangle = \sum_{a,b=1}^{6} \frac{a+b}{36} = 7.$$

$$\mathrm{Var}(X) = \sum_{a,b=1}^{6} \frac{(a+b)^2}{36} - 49 = \frac{1}{3}\sum_{a=1}^{6} a^2 + \frac{1}{18}\left(\sum_{a=1}^{6} a\right)^2 - 49 = \frac{91}{3} + \frac{441}{18} - 49 = \frac{35}{6}.$$

2. The Dirac δ-function

We will try now to introduce a probability density distribution for a deterministic random variable. Let us assume that $(\Omega, \mathcal{F}, \mathbb{P})$ is be a probability space and $X : \Omega \to \mathbb{R}$ is a deterministic RV taking only value x_0. Let us denote its, unknown for now, density by $\delta_{x_0}(x)$. Such density has to satisfy some special properties. For example, let us take any function $f\colon \mathbb{R} \to \mathbb{R}$ and consider new RV Y defined as $Y = f(X)$. By definition

$$\mathbb{E}[Y] = \int f(x)\delta_{x_0}(x)\, \mathrm{d}\, x = f(x_0).$$

Indeed, Y is a deterministic RV taking only value $f(x_0)$, which means that its average should be equal to $f(x_0)$. The relation above is usually used as a definition of Dirac δ-function. A Dirac δ-function is not a function in the common sense: no such a quantity can be defined rigorously as a function, rather $\delta_{x_0}(x)$ should be

intended as a *distribution*, i.e. it is defined by its action on a test function $f(x)$. This means that we are not allowed to talk about it as a function taking some arbitrary values, but only as a part of the integrand. However, below we list some properties of it that are similar to analogous ones for general functions but some of them are different.

DEFINITION 2.1. *We say that $\delta(x)$ is a Dirac δ-function if for any smooth and absolutely integrable function $f(x)$ on $\mathbb{R}$ we have*

$$\int_{-\infty}^{\infty} f(x)\delta(x)\,\mathrm{d}\,x = f(0). \tag{12}$$

The "shifted" δ-function $\delta_a(x)$ can be now simply written as $\delta(x_1 - a_1)$, so that for any function $f(x)$ we have

$$\int_{-\infty}^{\infty} f(x)\delta(x_1 - a_1)\,\mathrm{d}\,x = \int_{-\infty}^{\infty} f\left(x + a\right)\delta(x)\,\mathrm{d}\,x = f(a).$$

Now taking different test functions $f(x)$ we can obtain following properties of δ-function:

PROPOSITION 2.1. *Let $\delta(x)$ be a Dirac δ-function defined by (12), then:*

1. *The δ-function is normalized as a probability distribution, i.e. $\int_{-\infty}^{\infty}\delta(x)\,\mathrm{d}\,x = 1$.*
2. *If $g(x)$ has n simple real roots $x_1, ..., x_n$ then*

$$\delta(g(x)) = \sum_{j=1}^{n}\frac{\delta\left(x - x_j\right)}{\left|g'\left(x_j\right)\right|}. \tag{13}$$

In particular for $a \neq 0$ one has

$$\delta\left(ax\right) = \frac{1}{|a|}\delta(x).$$

3. *Let $\theta(x)$ be a Heaviside step function defined by*

$$\theta(x) = \begin{cases} 1 & \text{if} \quad x \geq 0, \\ 0 & \text{if} \quad x < 0. \end{cases}$$

Then

$$\int_{-\infty}^{x}\delta(y)\,\mathrm{d}\,y = \theta(x) \Rightarrow \delta(x) = \frac{\mathrm{d}\,\theta(x)}{\mathrm{d}\,x}, \tag{14}$$

where the derivative is taken in a distributional sense.

4. *Fourier transform and inverse Fourier transform of δ-function are given by*

$$\mathcal{F}\left[\delta\right](X) = \int_{-\infty}^{\infty}\delta(x)\,\mathrm{e}^{ixX}\,\mathrm{d}\,x = 1,$$

$$\mathcal{F}^{-1}\left[\delta\right](X) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\delta(x)\,\mathrm{e}^{-ixX}\,\mathrm{d}\,x = \frac{1}{2\pi}.$$

☞ Let us prove the formulas above. To prove that the integral of the δ-function is 1, it is enough to take $f(x) \equiv 1$ in (12).

Eq. (13) is proved by showing that both sides of the equation have the same effect inside an integration. Let us assume that there exist such n intervals $I_1 \sqcup I_2 \sqcup \ldots \sqcup I_n = \mathbb{R}$ that

- $g(x)$ is monotonic on every I_j, $j = 1, \ldots, n$;
- for every $j = 1, \ldots, n$ there is exactly one simple root of $g(x)$ that belongs to I_j.

Then for arbitrary absolutely integrable function $f(x)$ on $\mathbb{R}$ we have

$$\begin{aligned}\int\limits_{-\infty}^{\infty} f(x)\delta\left(g(x)\right)\mathrm{d}\,x &= \sum_{j=1}^{n}\int\limits_{I_j} f(x)\delta\left(g(x)\right)\mathrm{d}\,x \\ &\overset{s=g(x)}{=} \sum_{j=1}^{n}\int\limits_{I_j} f\left(g^{-1}(s)\right)\frac{\delta(s)\,\mathrm{d}\,s}{g'\left(g^{-1}(s)\right)} \\ &= \sum_{j=1}^{n}\frac{f\left(x_j\right)}{\left|g'\left(x_j\right)\right|} \\ &= \int\limits_{-\infty}^{\infty} f(x)\sum_{j=1}^{n}\frac{\delta\left(x-x_j\right)}{\left|g'\left(x_j\right)\right|}\,\mathrm{d}\,x.\end{aligned}$$

The first part of Eq. (14) is obvious after one takes $f(s) = \theta(x - s)$. Then

$$\int\limits_{-\infty}^{x}\delta(y)\,\mathrm{d}\,y = \int\limits_{-\infty}^{\infty} f(y)\delta(y)\,\mathrm{d}\,y = f(0) = \theta(x).$$

The second identity is proved by showing that both sides of the equation have the same effect inside an integration. Let $f(x)$ be an arbitrary absolutely integrable on $\mathbb{R}$. Then obviously $f(x) \to 0$ when $x \to \infty$. We have

$$\begin{aligned}\int\limits_{-\infty}^{\infty}\left(\delta(x) - \frac{\mathrm{d}\,\theta(x)}{\mathrm{d}\,x}\right)f(x)\,\mathrm{d}\,x &= f(0) - \theta(x)f(x)\big|_{-\infty}^{\infty} + \int\limits_{-\infty}^{\infty}\theta(x)f'(x)\,\mathrm{d}\,x \\ &= f(0) + \int\limits_{0}^{\infty} f'(x)\,\mathrm{d}\,x = f(0) + f(x)\big|_{0}^{\infty} = 0.\end{aligned}$$

Finally, the Fourier transform identities follow from the definition of δ-function.

The n-th derivative of $\delta(x)$ can be defined as a distribution on the set $C^{n+1}(\mathbb{R})$ by the identity

$$\int\limits_{-\infty}^{\infty} f(x)\delta^{(n)}(x)\,\mathrm{d}\,x = (-1)^n f^{(n)}(0).$$

This definition makes integration by parts valid while dealing with integrals containing δ-function.

The introduction of the Dirac δ-function allows us to introduce a density $\rho(x)$ also for deterministic and discrete RVs. Indeed,

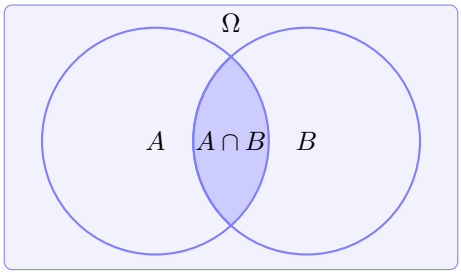
- if X is a deterministic RV taking only value x_0, then $\rho(x) = \delta(x - x_0)$.
- if X is a discrete RV taking values $\{x_i\}_{i=1}^n$ with probabilities $\{p_i\}_{i=1}^n$, then $\rho(x) = \sum_i p_i \delta(x - x_i)$.

3. Conditional probability

The conditional probability $\mathbb{P}[A|B]$ can be intended as the probability that the event $A \subset \Omega$ occurs given that the event $B \subset \Omega$ has already occurred. The so-called Bayes' Theorem follows directly from this definition, and it is given by the following expression.

DEFINITION 3.1. *The conditional probability* $\mathbb{P}[A|B]$ *of the event* A *given* B *is defined through Bayes' formula*

$$\mathbb{P}[A|B]\mathbb{P}[B] = \mathbb{P}[A \cap B].$$

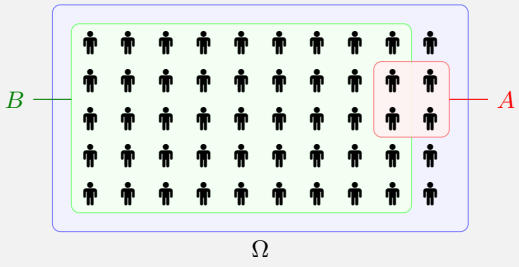


DEFINITION 3.2. *If the conditioning does not affect the marginal probability, then the two events are statistically independent*

$$\mathbb{P}[A|B] = \mathbb{P}[A] \Leftrightarrow \mathbb{P}[A \cap B] = \mathbb{P}[A]\mathbb{P}[B].$$

Using the above definition of conditional probability distribution, one can define conditional expectation, conditional moments, etc.

EXAMPLE Let us consider the following example. We have a population of individuals and we consider the event $A =$ sick individual and $B =$ vaccinated individual.



In the picture above

$$\mathbb{P}[A] = \frac{8}{100}, \qquad \mathbb{P}[B] = \frac{90}{100}, \qquad \mathbb{P}[A \cap B] = \frac{4}{100}$$

so that

$$\mathbb{P}[A|B] = \frac{4}{90} \approx 4.4\%$$

On the other hand

$$\mathbb{P}[A|B^c] = \frac{4}{10} = 40\%.$$

Observe also that $\mathbb{P}[B|A] = \frac{4}{8} = 50\%$: there is an important difference (qualitative and quantitative) between $\mathbb{P}[B|A]$ and $\mathbb{P}[A|B]$.

4. Multidimensional random variables

It is natural to consider experiments in which multiple outcomes occur at the same time, for example the observation of the positions of n particles after running some dynamical model. It is natural then to take $\Omega = \Omega_1 \times \Omega_2 \times \ldots \times \Omega_n$, where n is the number of such outcomes, Ω_j being the state space in which the jth outcome lives. We can then define a multidimensional distribution describing a multidimensional random variables.

DEFINITION 4.1. *Let $\Omega = \Omega_1 \times \Omega_2 \times \ldots \times \Omega_n$ be a state space for the probability space $(\Omega, \mathcal{F}, \mathbb{P})$. We then say that $\mathbb{P}$ defines joint probability distribution for the vector random variable $\boldsymbol{X} \colon \Omega \to \mathbb{R}^n$.*

In discrete settings this probability distribution is defined by probabilities $P_{\boldsymbol{X}}(\boldsymbol{x}) = \mathbb{P}[\boldsymbol{X} = \boldsymbol{x}]$, while in continuous setting we can introduce probability density $\rho_{\boldsymbol{X}}(\boldsymbol{x})$. Both quantities are non-negative and satisfy normalization $\sum_{\boldsymbol{x}} P_{\boldsymbol{X}}(\boldsymbol{x}) = 1$ in the discrete setting and $\int_{\boldsymbol{x}} \rho_{\boldsymbol{X}}(\boldsymbol{x}) \,\mathrm{d}\, \boldsymbol{x} = 1$ in the continuous one.

DEFINITION 4.2. *Starting from a joint probability, we can obtain the probability of the i-th component by summing over other components*

$$P_i(\omega) = \mathbb{P}[X_i = x] = \sum_{\boldsymbol{y}, y_i = x_i} P_{\boldsymbol{X}}(\boldsymbol{y}).$$

The quantity $P_i(x)$ is the marginal probability of X_i.

Analogously to the one dimensional case, we can introduce random variables, their averages and moments. For example the cumulative for the joint probability distribution will take a form

$$\Phi_{\boldsymbol{X}}(\boldsymbol{x}) = \mathbb{P}[X_1 \leq x_1, X_2 \leq x_2, \ldots, X_n \leq x_n],$$

and the density of joint distribution is given by

$$\rho_{\boldsymbol{X}}(\boldsymbol{x}) = \left[\prod_{i=1}^{n} \frac{\partial}{\partial x_i}\right] \Phi_{\boldsymbol{X}}(\boldsymbol{x}).$$

Finally, one can generalize the concept of δ-function to any dimension n by

DEFINITION 4.3. *We say that $\delta(\boldsymbol{x})$ is a n-dimensional Dirac δ-function if for any $\boldsymbol{x} \in \mathbb{R}^n$ we have*

$$\delta(\boldsymbol{x}) = \prod_{j=1}^{n} \delta(x_j).$$

The above definition yields that for any smooth and integrable function $f \colon \mathbb{R}^n \to \mathbb{R}$ we have

$$\int_{\mathbb{R}^n} f(\boldsymbol{x}) \delta(\boldsymbol{x}) = f\left(\boldsymbol{0}\right).$$

Given a multidimensional random variable, it is convenient to estimate how much the different components are "dependent" from each other. One way is to compute their *covariance*. For simplicity we restrict now ourselves to the case $n = 2$, the generic case being a straightforward generalisation.

DEFINITION 4.4. *Given a multidimensional RV $\boldsymbol{X} = (X_1, X_2)$, we define the covariance between X_1 and X_2 as*

$$\mathrm{Cov}[X_1, X_2] \coloneqq \mathbb{E}[X_1 X_2] - \mathbb{E}[X_1]\mathbb{E}[X_2] = \mathbb{E}[(X_1 - \mathbb{E}[X_1])\,(X_2 - \mathbb{E}[X_2])].$$

Suppose now that the variables are continuous and let $\rho_{\boldsymbol{X}}(x_1, x_2)$ be a density of the joint probability distribution for X_1, X_2, and $\rho_{X_j}(x)$ be corresponded marginal densities. Then by definition

$$\begin{aligned}\mathrm{Cov}[X_1, X_2] &= \iint x_1 x_2 \rho_{\boldsymbol{X}}(x_1, x_2)\,\mathrm{d}\,x_1\,\mathrm{d}\,x_2 - \int x\rho_{X_1}(x)\,\mathrm{d}\,x \int x\rho_{X_2}(x)\,\mathrm{d}\,x \\ &= \iint (x_1 - \mathbb{E}[X_1])\,(x_2 - \mathbb{E}[X_2])\,\rho_{\boldsymbol{X}}(x_1, x_2)\,\mathrm{d}\,x_1\,\mathrm{d}\,x_2.\end{aligned}$$

As anticipated, covariance is usually used to study the dependence (correlation) between two RVs.

DEFINITION 4.5. *Random variables whose covariance is zero are called uncorrelated.*

However one should distinguish between being statistically independent and uncorrelated. Independence implies absence of correlation, but not vice versa.

PROPOSITION 4.1. *Let X_1, X_2 be two statistically independent random variables defined on the same probability space. Then they are uncorrelated as well.*

PROOF. If X_1, X_2 are statistically independent, then

$$\rho_{\boldsymbol{X}}(x_1, x_2) = \rho_{X_1}(x_1)\rho_{X_2}(x_2),$$

that yields $\mathrm{Cov}[X_1, X_2] = \mathbb{E}[X_1 X_2] - \mathbb{E}[X_1]\mathbb{E}[X_2] = \mathbb{E}[X_1]\mathbb{E}[X_2] - \mathbb{E}[X_1]\mathbb{E}[X_2] = 0$. □

If nulle covariance is an indicator of absence of correlation, covariance itself is not a proper measure of the correlation between RVs. A true indicator of dependence is so called correlation coefficient, which rescale the covariance by the size of the fluctuations of each of the factors involved in its definition.

DEFINITION 4.6. *Let X_1, X_2 be two random variables defined on the same probability space. Then we define their correlation coefficient by*

$$\varrho_{X_1, X_2} = \frac{\mathrm{Cov}[X_1, X_2]}{\sqrt{\mathrm{Var}[X_1]\,\mathrm{Var}[X_2]}}.$$

PROPOSITION 4.2. *Let X_1, X_2 be two random variables defined on the same probability space. Then*

$$|\varrho_{X_1, X_2}| \leq 1,$$

moreover $\varrho_{X1, X_2} = 1$ corresponds to perfect positive linear relationship and $\rho_{X_1, X_2} = -1$ corresponds to perfect negative linear relationship.

In the case of general multidimensional RV it is natural to consider all pairwise correlations between coordinates.

DEFINITION 4.7. *Let $\boldsymbol{X}$ be a multidimensional RV. Its covariance matrix $\boldsymbol{C_X}$ is the real symmetric matrix whose entries*

$$C_{ij} = \mathrm{Cov}\left(X_i, X_j\right).$$

PROPOSITION 4.3. *For any multidimensional RV its covariance matrix $\boldsymbol{C_X}$ is non-negative definite, i.e. for any $\boldsymbol{x} \in \mathbb{R}^n$*

$$\langle \boldsymbol{x}, \boldsymbol{C_X x} \rangle \geq 0,$$

or equivalently all the eigenvalues of $\boldsymbol{C_X}$ are real and non-negative.

Let us also note that the diagonal elements are $C_{ii} = \mathrm{Var}\left(X_i\right)$. If all coordinates X_i's are statistically independent, then $\boldsymbol{C_X}$ is a diagonal matrix. Analogously one can define correlation matrix as the matrix whose entries are correlations coefficients.

5. A list of relevant random variables

☞ THE DISCRETE DELTA Let X be a discrete RV taking integer values with probabilities

$$P_X(n) = \delta_{n,n_0} \qquad n \in \mathbb{N}.$$

meaning that it takes a certain value n_0 with probability 1 and all other values with probability 0 (i.e. it is certain that its value is n_0). This random variable behaves as a "discrete δ-function". In particular

- $\langle X \rangle = n_0$.
- $\mathrm{Var}(X) = 0$.
- $M_X\left(t\right) = \mathrm{e}^{n_0 t}$ and $\chi_X\left(t\right) = \mathrm{e}^{i n_0 t}$.

☞ POISSON RANDOM VARIABLE Let X be a discrete RV taking non-negative integer values with probabilities

$$P_X(n) = \frac{\lambda^n \, \mathrm{e}^{-\lambda}}{n!} \qquad n \in \mathbb{N}.$$

This is said to be a *Poisson random variable with parameter* λ. It has the following properties

- $\langle X \rangle = \lambda$.
- $\mathrm{Var}(X) = \lambda$.
- $M_X\left(t\right) = \mathrm{e}^{\lambda\left(\mathrm{e}^t - 1\right)}$, $\chi_X\left(t\right) = \mathrm{e}^{\lambda\left(\mathrm{e}^{it} - 1\right)}$.

☞ BERNOULLI RANDOM VARIABLE Let X be a discrete RV taking values $\{0, 1\}$ with probabilities

$$P_X(1) = p, \qquad P_X(0) = 1 - p.$$

or equivalently

$$P_X(n) = p\delta_{n,1} + (1-p)\delta_{n,0}.$$

This is a *Bernoulli random variable* and it has the following properties.

- $\langle X \rangle = p$.
- $\mathrm{Var}(X) = p\left(1-p\right)$.
- $M_X\left(t\right) = 1 + p\left(\mathrm{e}^t - 1\right)$ and $\chi_X\left(t\right) = 1 + p\left(\mathrm{e}^{it} - 1\right)$.

☞ Exponential random variable We say that continuous RV X has *exponential distribution* with parameter λ if its density is given by

$$\rho(x) = \begin{cases} \lambda \mathrm{e}^{-\lambda x}, & \text{if } x \geq 0, \\ 0, & \text{if } x < 0. \end{cases} \tag{15}$$

Such variable has the following properties:

- $\langle X \rangle = \frac{1}{\lambda}$.
- $\mathrm{Var}(X) = \frac{1}{\lambda^2}$.
- $\langle X^p \rangle = \frac{p!}{\lambda^p}$.
- $M_X(t) = \frac{\lambda}{\lambda - t}$ for $\lambda < t$, and $\chi_X(t) = \frac{\lambda}{\lambda - it}$.

☞ Gaussian random variable We say that the continuous RV X has a normal (Gaussian) distribution with average μ and variance σ^2 if its density is given by

$$\rho(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \mathrm{e}^{-\frac{(x-\mu)^2}{2\sigma^2}} \qquad x \in \mathbb{R}. \tag{16}$$

We write that $X \sim \mathcal{N}(\mu, \sigma^2)$. A Gaussian random variable has the following properties

- $\langle X \rangle = \mu$.
- $\mathrm{Var}(X) = \sigma^2$.
- $M_X(t) = \mathrm{e}^{\mu t + \frac{1}{2}\sigma^2 t^2}$ and $\chi_X(t) = \mathrm{e}^{i\mu t - \frac{1}{2}\sigma^2 t^2}$.

The normal distribution is a fundamental distribution mostly due to the central limit theorem. Roughly speaking, the theorem says that if we have a set $\{X_i\}_{i=1}^n$ of random variables which are independent and have the same distribution with mean μ and finite variance σ^2, given their average $Z_n \coloneqq \frac{1}{n}\sum_{i=1}^n X_i$, then $Z_n \xrightarrow{n \to +\infty} \mathcal{N}(\mu, \sigma^2/n)$. Physical quantities that are expected to be the sum of many independent processes (such as measurement errors) often have distributions that are nearly normal. Moreover, many results and methods (such as propagation of uncertainty and least squares parameter fitting) can be derived analytically in explicit form when the relevant variables are normally distributed.

☞ Multivariate Gaussian distribution We say that multidimensional continuous RV $\boldsymbol{X}$ has a normal (Gaussian) distribution with mean vector $\boldsymbol{\mu}$ and positive definite covariance matrix $\boldsymbol{\Sigma}$ if its density is given by

$$\rho(\boldsymbol{x}) = \frac{1}{\sqrt{2\pi \det \boldsymbol{\Sigma}}} \mathrm{e}^{-\frac{1}{2}\left\langle \boldsymbol{x}-\boldsymbol{\mu}, \boldsymbol{\Sigma}^{-1}(\boldsymbol{x}-\boldsymbol{\mu}) \right\rangle} \qquad \boldsymbol{x} \in \mathbb{R}^n.$$

It has the following properties.

- All marginal distributions of $\boldsymbol{X}$ are also Gaussian.
- Every RV variable X_j is a Gaussian RV with mean μ_j and variance Σ_{jj}.
- The covariance of X_i and X_j is given by $\Sigma_{i,j}$, while the correlation is given by $\frac{\Sigma_{ij}}{\sqrt{\Sigma_{ii}\Sigma_{jj}}}$.
- $M_{\boldsymbol{X}}(\boldsymbol{t}) = \mathrm{e}^{\langle \boldsymbol{t}, \boldsymbol{\mu} \rangle + \frac{1}{2}\langle \boldsymbol{t}, \boldsymbol{\Sigma t} \rangle}$ and $\chi_{\boldsymbol{X}}(\boldsymbol{t}) = \mathrm{e}^{i\langle \boldsymbol{t}, \boldsymbol{\mu} \rangle - \frac{1}{2}\langle \boldsymbol{t}, \boldsymbol{\Sigma t} \rangle}$.

The computation of higher moments of a multivariate Gaussian distributed random variable can be performed using Wick's theorem. Wick's theorem is a method in Quantum Field Theory of reducing high-order derivatives to a combinatorics problem. This result allows to calculate high-order moments by using values of second order moments. Formally

THEOREM 5.1. *Let $\boldsymbol{X}$ be distributed according to multivariate Gaussian distribution with zero mean vector $\boldsymbol{\mu} = \mathbf{0}$ and covariance matrix $\boldsymbol{\Sigma}$. Then for any even sized set of indexes $(j_1, j_2, \dots, j_{2k}) \subset \{1, \dots, n\}^{2m}$*

$$\langle X_{j_1} X_{j_2} \dots X_{j_{2k}} \rangle = \sum_{\sigma \in \mathcal{P}_{2k}} \prod_{m=1}^{k} \left\langle X_{j_{\sigma(2m-1)}} X_{j_{\sigma(2m)}} \right\rangle,$$

where summation in σ runs over all pairings $\mathcal{P}_{2k}$ of $(j_1, j_2, \dots, j_{2k})$.

For example, if $X \sim \mathcal{N}\left(0, \sigma^2\right)$, then $\left\langle X^2 \right\rangle = \sigma^2$. Let us calculate $\left\langle X^6 \right\rangle$. We can write it as

$$\begin{aligned}\langle X\,X\,X\,X\,X\,X \rangle &= \sum_{\sigma \in P_6} \langle X\,X \rangle \langle X\,X \rangle \langle X\,X \rangle \\ &= \sigma^6 \#\left\{\text{pairings of } 1,2,3,4,5,6\right\} = 15\sigma^6.\end{aligned}$$

☞ DETERMINISTIC RV AS A LIMIT OF GAUSSIAN RV As discussed earlier, one can define deterministic RV as a continuous RV with density given by δ-function. However, the δ-function is not a proper function in a wide sense and some calculations with deterministic RV will need some justifications. One of the ways is to derive a "limiting" formula for the δ-function. In particular, one possibility is to take a zero-average normal distribution and send its variance/width to zero, i.e., write

$$\delta(x) = \lim_{\sigma \to 0} p_\sigma(x), \qquad p_\sigma(x) = \frac{1}{\sqrt{2\pi\sigma^2}}\, \mathrm{e}^{-\frac{x^2}{2\sigma^2}}.$$

This definition is also not proper definition of a function as one can check

$$\lim_{\sigma \to 0} p_\sigma(x) = \begin{cases} 0, & x \neq 0, \\ \infty, & x = 0. \end{cases}$$

However, we realize that $\delta(x)$ only serves to calculate averages; it only has a meaning inside an integration. If we adopt the convention that one should set $\sigma \to 0$ in above only *after* performing corresponding integration, we can use above for our calculations. For example,

$$\int_{-\infty}^{\infty} \delta(x) f(x)\, \mathrm{d}\, x = \lim_{\sigma \to 0} \int_{-\infty}^{\infty} p_\sigma(x) f(x)\, \mathrm{d}\, x = \lim_{\sigma \to 0} \int_{-\infty}^{\infty} \frac{\mathrm{d}\, x}{\sqrt{2\pi}}\, \mathrm{e}^{-x^2/2} f(\sigma x) = f(0).$$

$$\begin{aligned}\int_{-\infty}^{\infty} \delta'(x) f(x) &= \lim_{\sigma \to 0} \int_{-\infty}^{\infty} \left\{ \frac{\mathrm{d}}{\mathrm{d}\, x}\Big(p_\sigma(x) f(x)\Big) - p_\sigma(x) f'(x) \right\} \\ &= \lim_{\sigma \to 0} p_\sigma(x) f(x)\big|_{-\infty}^{\infty} - f'(0) = -f'(0).\end{aligned}$$

Exercises

(1) Calculate following integrals
   (a) $\int_{-\infty}^{\infty} 7\delta(x)\,\mathrm{e}^{-x^2}\cos x\,\mathrm{d}\,x$.
   (b) $\int_{-5}^{5}\left(x^2+2x+1\right)\delta\left(x-1\right)\mathrm{d}\,x$.
   (c) $\int_{0}^{\infty}\left(\cos\left(3x\right)+2\right)\delta\left(x-\pi\right)\mathrm{d}\,x$.
   (d) $\int_{-1}^{1}\mathrm{e}^{-x^2}\cos(x)\delta\left(x-2\right)\mathrm{d}\,x$.

(2) Let $f:\mathbb{R}\to\mathbb{R}$ be a deterministic, smooth enough function. Assume that it has finitely many distinct simple zeros $(x_1,x_2,\ldots,x_n)\subset\mathbb{R}$. Prove the *Kac–Rice formula*

$$\{\text{Number of zeros of } f(x) \text{ in } (a,b)\} = \int_a^b \delta\left(f(x)\right)\left|f'(x)\right|\mathrm{d}\,x.$$

(3) Let X_1 and X_2 be continuous random variables with joint probability density function

$$p\left(x_1,x_2\right) = k\left(1-x_1x_2^2\right), \quad x_1,x_2\in[0,1].$$

   (a) Find the value of k.
   (b) Calculate the marginal densities $p_{X_1}(x)$ and $p_{X_2}(x)$.
   (c) Calculate the corresponding marginal means.
   (d) Are X_1 and X_2 independent?
   (e) Find the covariance between X_1 and X_2.
   (f) Calculate the conditional density of X_2 given $X_1 = 1/3$.

(4) A diagnostic test for a disease is such that it (correctly) detects the disease in 90% of the individuals who actually have the disease. Also, if a person does not have the disease the test will report that he or she does not have it with probability 0.9. Only 1% of the population has the disease in question. If a person is chosen at random from the population and the diagnostic test indicates that she has the disease, what is the conditional probability that she does in fact have the disease? Would you call this diagnostic test reliable?

(5) Assume that Y is Normally distributed such that $Y\sim\mathcal{N}\left(\mu,\sigma^2\right)$. After observing a value Y a mathematician constructs a rectangle with length $L=|Y|$ and width $W=3\,|Y|$. Let A denote the area of the resulting rectangle. What is the expected area $\langle A\rangle$?

(6) Consider the bi-variate Gaussian distribution defined by the density

$$P_2\left(x_1,x_2\right) = \sqrt{\frac{1-\lambda^2}{\left(2\pi\sigma^2\right)^2}}\exp\left\{-\frac{1}{2\sigma^2}\left(x_1^2-2\lambda x_1x_2+x_2^2\right)\right\},$$

where the parameter $\lambda\in(-1,1)$ is such to ensure that the quadratic form in the exponent is positive definite. To fix ideas, one may interpret $P_2\left(x_1,x_2\right)$ as the Boltzmann distribution of two harmonic oscillators coupled by a potential term proportional to x_1x_2.
   (a) Verify that this is well normalized by direct integration or by comparing our distribution with the zero-mean multidimensional Gaussian

distribution

$$P(\boldsymbol{x}) = \sqrt{\frac{(2\pi)^N}{\det \boldsymbol{A}}}\, \mathrm{e}^{-\frac{1}{2}\langle \boldsymbol{x}, \boldsymbol{A}\boldsymbol{x}\rangle} \quad \text{where} \quad \boldsymbol{A} = \begin{pmatrix} 1 & -\lambda \\ -\lambda & 1 \end{pmatrix}.$$

(b) Verify that the marginal probability of the individual variables is

$$P_1(x) = \frac{1}{\sqrt{2\pi\sigma_\lambda^2}}\, \mathrm{e}^{-\frac{x^2}{2\sigma_\lambda^2}} \quad \text{with} \quad \sigma_\lambda^2 = \frac{\sigma^2}{1-\lambda^2}.$$

Verify that σ_λ^2 is the variance $\langle\!\langle x_1^2 \rangle\!\rangle \coloneqq \langle x_1^2 \rangle - \langle x_1 \rangle^2$.

(c) Show that the covariance of x_1 and x_2 is

$$\langle\!\langle x_1 x_2 \rangle\!\rangle \coloneqq \langle x_1 x_2 \rangle - \langle x_1 \rangle \langle x_2 \rangle = \lambda \sigma_\lambda^2.$$

(d) Often it is convenient to calculate the normalised variance, or *correlation coefficient*,

$$\rho \coloneqq \frac{\langle\!\langle x_1 x_2 \rangle\!\rangle}{\sqrt{\langle\!\langle x_1^2 \rangle\!\rangle \langle\!\langle x_2^2 \rangle\!\rangle}}.$$

Show that this is merely given by λ. Therefore the parameter λ in the distribution is a measure of how correlated the variables x_1 and x_2 are. Note that in the limit $\lambda \to 0$ the variables are not correlated at all and the distribution factorizes

$$P_2(x_1, x_2)|_{\lambda=0} = P_1(x_1) P_1(x_2).$$

In the limit $\lambda \to 1$ the variables are maximally correlated and the distribution becomes a function of $x_1 - x_2$ but it is not normalisable anymore. We can now interpret the increase of the variance with λ: the correlation between the variables allow them to take arbitrarily large values, with the only restriction of their difference being small.

(e) By using Bayes rule show that

$$P_{1|1}(x_1|x_2) = \frac{P_2(x_1, x_2)}{P_1(x_2)} = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left\{ -\frac{1}{2\sigma^2} (x_1 - \lambda x_2)^2 \right\}.$$

Then, at $\lambda = 0$ (no correlation) the values taken by x_1 are independent of x_2, while for $\lambda \to 1$ they are centred around those taken by x_2, and hence strongly conditioned by them.

LECTURE 5

Probability (continue)

1. Foundations of Information Theory

We would like to develop a usable measure of the information we get from observing the occurrence of an event E having probability $p = \mathbb{P}[E]$. Our first reduction will be to ignore any particular features of the event, and only observe whether or not it happened. Thus we will think of an event as the observance of a symbol whose probability of occurring is p. We will thus be defining the information in terms of the probability p.

The approach we will be taking here is axiomatic: below is a list of the four fundamental axioms we will use to define our *information measure* $I(p)$:

(1) Information is a non-negative quantity: $I(p) \geq 0$.
(2) If an event has probability 1, we get no information from the occurrence of the event, $I(1) = 0$.
(3) If two independent events E_1 and E_2 occur, then the information we get from observing the events is the sum of the two informations,
$$I(\mathbb{P}[E_1 \cap E_2]) = I(\mathbb{P}[E_1]) + I(\mathbb{P}[E_2]).$$
(4) We will want our information function I to be a continuous, and, in fact, monotonic function of the probability, so that slight changes in probability should result in slight changes in information.

It is possible to show that the requirement above are compatible with the form
$$I(p) = -\log_a(p)$$
for some positive constant a. The base a determines the units we are using.

1.1. Shannon entropy. The probability distribution $\mathbb{P}$ of a RV X is a tool to quantify the "information content" of the possible values X it can assume. If we consider the state of a RV as a "message" communicated between a sender and a receiver, one could ask: *which is the average amount of information needed to specify this message?* Let us use the shorthand notation $p(x) \coloneqq \mathbb{P}[X = x]$ in the following. We thus need to define a measure, $H_X[p]$ of the information content, with the following properties

(1) H_X is a monotonic decreasing function of $p(x)$. In fact, the information can be seen as the "degree of surprise" on learning the state of X: the more an event is unlikely, the more information we discover, while if an event occurs almost certainly, the gain of information is really low.
(2) H_X is additive if two events are statistically independent, i.e. the total information is simply the sum $H_{X+Y} = H_X + H_Y$ whenever $\mathbb{P}[X = x, Y = y] = \mathbb{P}[X = x]\mathbb{P}[Y = y]$.

DEFINITION 1.1. *Let X be a discrete random variable defined on the probability space $(\Omega, \mathcal{F}, \mathbb{P})$. We define its Shannon entropy H_X by*

$$H_X[p] = -\sum_x p(x) \log_2 p(x) = -\mathbb{E}[\log_2 p(x)],$$

where we define by continuity $0 \log_2 0 = 0$.

In this section we use the logarithm with base 2, which is well adapted to digital communication, and the entropy is then expressed in *bits*. The choice of the basis for the log is arbitrary: the most common convention is $\log_2$. One can switch to natural logarithms ln and the definition differs simply of a factor $\ln 2$, i.e.

$$H_X[p] = -\frac{1}{\ln 2} \sum_x p(x) \log_2 p(x) \tag{17}$$

In this way, the information is measured in *nats*, natural digits.

When there is no ambiguity we use H instead of H_X. Intuitively, the entropy gives a measure of the uncertainty of the random variable. It is sometimes called the missing information: the larger the entropy, the less a priori information one has on the value of the random variable. This measure is roughly speaking the logarithm of the number of typical values that the variable can take, as the following examples show.

EXAMPLE A fair coin has two values with equal probability. Its entropy is 1 bit.

EXAMPLE Imagine throwing M fair coins: the number of all possible outcomes is 2^M. The entropy equals M bits.

EXAMPLE A fair dice with n faces has entropy $\log_2 n$.

EXAMPLE DNA is built from a sequence of bases which are of four types, A, T, G, C. In natural DNA of primates, the four bases have nearly the same frequency, and the entropy per base, if one makes the simplifying assumptions of independence of the various bases, is $H = -\log_2(1/4) = 2$. In some genera of bacteria, one can have big differences in concentrations: $p(G) = p(C) = 0.38, p(A) = p(T) = 0.12$, giving a smaller entropy $H \simeq 1.79$.

DEFINITION 1.2. *Let X be a continuous random variable defined on probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with density $\rho(x)$. We define its Shannon entropy H_X by*

$$H_X[\rho] = -\int_{\mathbb{R}} \rho(x) \log_2 \rho(x) \, \mathrm{d}\, x.$$

THEOREM 1.1 (Properties of Shannon entropy). *For any random variable X its Shannon entropy satisfies the following properties.*

1. *$H_X \geq 0$ with the equality iff X is a deterministic RV, i.e. $\rho(x) = \delta(x - c)$ for some c.*

(2) *if X is a deterministic RV on a probability space $(\Omega, \mathcal{F}, \mathbb{P})$ with $|\Omega| = n$, then $H_X \leq \log_2 n$ with the equality holding iff $p(x) \equiv \frac{1}{n}$ for any feasible x, i.e. uniform distribution.*

1.2. Statistical Inference. "Entropy" is a key concept in information theory and has several applications in the context of Statistical Inference. This name denotes a broad class of problems where a set of data x is given but $p(x)$ is either unknown or not completely specified and the task is thus to estimate it. Assume for example that the "true" distribution $p(x)$ is infeasible to evaluate exactly, thus we describe it by some approximating distribution $q(x)$: what is the additional amount of information required to specify the state of x by means of $q(x)$? The answer is provided by the *relative entropy* of the distributions $p(x)$ and $q(x)$ (or *Kullback-Leibler divergence*) $\mathrm{KL}(p\|q)$ which is a measure of the dissimilarity between $p(x)$ and $q(x)$, thus one usually tries to improve the approximation by minimizing the KL divergence. This is defined as:

DEFINITION 1.3. *The Kullback-Leibler divergence between two discrete probability distributions $p(x)$ and $q(x)$ over the same finite space Ω is defined as*

$$\mathrm{KL}(p\|q) = \sum_x p(x) \log_2 \frac{p(x)}{q(x)},$$

where we adopt the conventions $0 \log 0 = 0$, $0 \log(0/0) = 0$.

One can show that KL divergence have the following properties

THEOREM 1.2. *Let $p(x)$ and $q(x)$ be two discrete probability distributions over the same finite space Ω. Then*

(1) $\mathrm{KL}(p\|q)$ *is convex in $p(x)$;*
(2) $\mathrm{KL}(p\|q) \geq 0$ *with equality holding only for $p(x) \equiv q(x)$.*

This theorem follows from the convexity of function $f(x) = -\log_2 x$ and Jensen's inequality. The KL divergence $\mathrm{KL}(p\|q)$ thus looks like a distance between the probability distributions p and q, although it is not symmetric. A symmetrised version is provided by the so-called Jeffrey's divergence

$$J(p\|q) = \frac{\mathrm{KL}(p\|q) + \mathrm{KL}\,(q||p)}{2}.$$

1.3. Maximum-entropy distributions. Suppose that some detail on $p(x)$ is available. For example we may have an estimate $h^\star$ for the average value $\mathbb{E}[h(X)]$ of some function h. The task is to fully characterise $p(x)$ starting from that average. Recall that the "entropy" of x is the degree of surprise on learning its state, thus it quantifies our ignorance about x, how uncertain are in average the observations of x. In light of that, a principle often applied in statistical inference is the *Maximum Entropy Principle* (MaxEnt).

The best estimate for $p(x)$ is the one that maximizes $H_X[p]$ and is compatible with the available knowledge on X (i.e. subject to the constraints given by $\mathbb{E}[h(X)]$). This estimate is believed to be the best one as it is the most unbiased, the one that prevents us from inappropriate assumptions. Let us now derive the $p(x)$ satisfyng the MaxEnt principle. We have to find

$$p_\star(x) = \arg\max_p H_X[p]$$

subject to the constraints

$$\sum_x p(x) = 1 \qquad h^\star = \mathbb{E}[h(x)] = \sum_x p(x)h(x).$$

We write $H[p] = -k\sum_x p(x)\ln p(x)$, where $k = \frac{1}{\ln 2}$. Such a problem can be solved by the *method of Lagrange multipliers*. We thus introduce two quantities, called Lagrange multipliers, λ_0 and λ_1, which allow us to translate our constrained maximization problem into an unconstrained one for

$$H_X[p;\lambda_0,\lambda_1] \coloneqq H[p] + k\lambda_0\left(\sum_x p(x) - 1\right) + k\lambda_1\left(\sum_x p(x)h(x) - h^\star\right).$$

The maximizing distribution is found by solving

$$\begin{cases} \frac{\partial}{\partial p(x)} H_X[p;\lambda_0,\lambda_1] & \implies \ln p(x) = -1 + \lambda_0 + \lambda_1 h(x) \\ \frac{\partial}{\partial \lambda_0} H_X[p;\lambda_0,\lambda_1] = 0 & \implies \sum_x p(x) = 1 \\ \frac{\partial}{\partial \lambda_1} H_X[p;\lambda_0,\lambda_1] = 0 & \implies \sum_{x\in A} p(x)h(x) = h^\star. \end{cases}$$

From the first equation it can be seen that

$$p(x) = \exp\left(\lambda_0 + \lambda_1 h(x) - 1\right) = \frac{1}{Z}\exp\left(\lambda_1 h(x)\right),$$

where $Z = \exp(1-\lambda_0)$ must be equal to $Z = \sum_x \exp(\lambda_1 h(x))$ because of the normalisation constraints, i.e., $\lambda_0 = 1 - \ln Z$,. Finally, λ_1 is chosen by enforcing the requirement on average and such as to satisfy

$$\sum_x p(x)h(x) = \frac{\partial \ln Z}{\partial \lambda_1} = h^\star$$

Note that since $H_X[p]$ is a strictly concave function, the solution of this optimization problem is unique and consists of a maximum.

1.4. Generalizations to many variables systems. More in general, we may have a vectorial random variable $\boldsymbol{X} = (X_1, \dots, X_N)$ and we may know the expected values $h^\star_\mu$ of specific measurements $h_\mu(\boldsymbol{X})$, with $\mu = 1, \dots, K$, that we will denote briefly $\boldsymbol{h}(\boldsymbol{X}) = (h_1(\boldsymbol{x}), \dots, h_K(\boldsymbol{x}))$. The maximum-entropy distribution subject to the constraints $\sum_{\boldsymbol{x}} p(\boldsymbol{x}) = 1$ and $\sum_{\boldsymbol{x}} p(\boldsymbol{x})h_\mu(\boldsymbol{x}) = h^\star_\mu$ for all $\mu = 1, \dots, K$ is found again by the Lagrange maximisation method now involving $K+1$ Lagrange parameters $\{\lambda_\mu\}_{\mu=0}^K$, K of which corresponding to the imposed constraints and with λ_0 representing the normalisation requirement $\sum_{\boldsymbol{x}} p(\boldsymbol{x}) = 1$. The condition to impose for each $p(\boldsymbol{x})$ is then

$$\frac{\partial}{\partial p(\boldsymbol{x})}\Big[H_{\boldsymbol{X}}[p] - \lambda_0\Big(1 - \sum_{\boldsymbol{x}} p(\boldsymbol{x})\Big) - \sum_{\mu=1}^K \lambda_\mu\Big(h^\star_\mu - \sum_{\boldsymbol{x}} p(\boldsymbol{x})h_\mu(\boldsymbol{x})\Big)\Big] = 0$$

where $H_{\boldsymbol{X}}[p] = -k\sum_{\boldsymbol{x}} p(\boldsymbol{x})\ln p(\boldsymbol{x})$. The solution of these latter equations takes the form

$$p(\boldsymbol{x}) = \frac{\mathrm{e}^{\sum_{\mu=1}^K \lambda_\mu h_\mu(\boldsymbol{x})}}{Z}, \qquad Z = \sum_{\boldsymbol{x}} \mathrm{e}^{\sum_{\mu=1}^K \lambda_\mu h_\mu(\boldsymbol{x})} \tag{18}$$

in which the parameters $\{\lambda_1, \dots, \lambda_K\}$ are found by solving the coupled equations

$$\forall \mu \in \{1, \dots, K\}: \qquad h^\star_\mu = \frac{\partial \ln Z}{\partial \lambda_\mu} = \frac{1}{Z}\sum_{\boldsymbol{x}} h_\mu(\boldsymbol{x})\,\mathrm{e}^{\sum_{\mu=1}^K \lambda_\mu h_\mu(\boldsymbol{x})}.$$

Solving the equation above, whether analytically or numerically, can unfortunately be quite difficult. The distribution (18) denotes the ensemble of microscopic configurations $\boldsymbol{x}$ compatible with prescribed averages of macroscopic observables $\boldsymbol{h}(\boldsymbol{X})$ and is often referred to as the *exponential model* in statistics and the *canonical ensemble* in the statistical mechanical gergon. The normalizing constant Z is called, in the statitical mechanical gergon, the *partition function* and denotes the effective number of microscopic configurations $\boldsymbol{x}$ compatible with the imposed values of the ensemble averages of $\boldsymbol{h}(\boldsymbol{X})$.

In canonical ensembles we tend to regard the probabilities $p(\boldsymbol{x})$ as parametrised directly by the vector $\boldsymbol{\lambda} = (\lambda_1, \ldots, \lambda_K)$. We no longer view these latter parameters as unknown complicated functions of the values $\boldsymbol{h}^\star$ and we simply write

$$p(\boldsymbol{x}) = \frac{\mathrm{e}^{\langle \boldsymbol{\lambda}, \boldsymbol{h}(\boldsymbol{x})\rangle}}{Z(\boldsymbol{\lambda})}, \qquad Z(\boldsymbol{\lambda}) = \sum_{\boldsymbol{x}} \mathrm{e}^{\langle \boldsymbol{\lambda}, \boldsymbol{h}(\boldsymbol{x})\rangle}$$

Observe that in the above derivation we should in principle have included also the inequality constraints $p(\boldsymbol{x}) \geq 0$ for all $\boldsymbol{x}$ when maximising the Shannon entropy – after all, probabilities are not allowed to be negative. However, it turned out in both cases that even without imposing them explicitly, the inequality constraints are satisfied automatically by the maximum entropy distributions we obtained.

1.4.1. *Microcanonical ensembles.* The so-called *microcanonical* ensembles refers to ensembles where the constraints are not only satistified on average, but by *each* configuration $\boldsymbol{x}$ of the ensemble i.e., $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{h}^\star \ \forall \boldsymbol{x}$. Clearly in this case

$$p(\boldsymbol{x}) = \frac{\delta_{\boldsymbol{h}(\boldsymbol{x}), \boldsymbol{h}^\star}}{Z} \qquad Z = \sum_{\boldsymbol{x}} \delta_{\boldsymbol{h}(\boldsymbol{x}), \boldsymbol{h}^\star}.$$

1.4.2. *Averages, fluctuations and susceptibilities.* Once the parameter values $\boldsymbol{\lambda}$ of the canonical ensemble are gieven, one can use the corresponding probability distribution $p(\boldsymbol{x})$ to estimate the value of any observable $\varphi(\boldsymbol{x})$ by calculating the ensemble average

$$\mathbb{E}[\varphi(\boldsymbol{x})] = \frac{\sum_{\boldsymbol{x}} \varphi(\boldsymbol{x})\, \mathrm{e}^{\langle \boldsymbol{\lambda}, \boldsymbol{h}(\boldsymbol{x})\rangle}}{Z(\boldsymbol{\lambda})}$$

In particular, remember that the expectation values for the key observables $h_\mu(\boldsymbol{x})$ can all be written as partial derivatives of the quantity $\Phi(\boldsymbol{\lambda}) = \ln Z(\boldsymbol{\lambda})$, which apparently acts as a generating function. In the terminology of statistical physics the quantity $\Phi(\boldsymbol{\lambda})$ would, apart from an overall multiplicative constant, be called the 'free entropy'. For the fluctuations in the key observables we have

$$\begin{aligned}
\mathrm{Var}[h_\mu(\boldsymbol{X})] &= \mathbb{E}[h_\mu^2(\boldsymbol{X})] - \big(\mathbb{E}[h_\mu(\boldsymbol{X})]\big)^2 \\
&= \frac{1}{Z(\boldsymbol{\lambda})} \sum_{\boldsymbol{x}} h_\mu^2(\boldsymbol{x})\, \mathrm{e}^{\langle \boldsymbol{\lambda}, \boldsymbol{h}(\boldsymbol{x})\rangle} - \Big(\frac{1}{Z(\boldsymbol{\lambda})} \frac{\partial Z(\boldsymbol{\lambda})}{\partial \lambda_\mu}\Big)^2 \\
&= \frac{1}{Z(\boldsymbol{\lambda})} \frac{\partial^2 Z(\boldsymbol{\lambda})}{\partial \lambda_\mu^2} - \frac{1}{Z^2(\boldsymbol{\lambda})} \left(\frac{\partial Z(\boldsymbol{\lambda})}{\partial \lambda_\mu}\right)^2 \\
&= \frac{\partial}{\partial \lambda_\mu} \left(\frac{1}{Z(\boldsymbol{\lambda})} \frac{\partial Z(\boldsymbol{\lambda})}{\partial \lambda_\mu}\right) = \frac{\partial^2 \Phi(\boldsymbol{\lambda})}{\partial \lambda_\mu^2}
\end{aligned}$$

From the above relations it also follows that

$$\mathrm{Var}[h_\mu(\boldsymbol{X})] = \frac{\partial}{\partial \lambda_\mu} \mathbb{E}[h_\mu(\boldsymbol{X})].$$

The latter quantity is called *susceptibility*; it measures the sensitivity of $\mathbb{E}[h_\mu(\boldsymbol{X})]$ to changes in its associated control variable λ_μ. All identities derived so far rely solely on the exponential dependence of the probabilities on the control parameters.

1.4.3. *Gibbs-Boltzmann distribution.* The concept of "entropy" in physics was introduced much earlier by Boltzmann in equilibrium thermodynamics as a measure of the "disorder" of a physical state of matter.

Consider a physical system at a certain temperature $T > 0$ and with a set of possible configurations $\boldsymbol{x}$, and let it evolve in time: after a while, it reaches a so called "thermal equilibrium" state and its properties (e.g., its energy) just fluctuate around constant average values. A basic assumption of statistical mechanics is that the "thermal equilibrium" of a system is the one that maximises the entropy.

It is reasonable to assume that this asymptotic macroscopic state is the one for which the number of compatible microscopic configurations (i.e. the multiplicity) is maximum. We can then find the equilibrium probability distribution by maximizing the thermodynamical entropy under the constraints of normalization and some fixed energy level (i.e. some fixed macroscopic average)

$$E = \sum_{\boldsymbol{x}} p(\boldsymbol{x})\mathcal{H}(\boldsymbol{x})$$

where $H(\boldsymbol{x})$ is a function of the configuration $\boldsymbol{x}$ that contains all the contributions to the overall energy (interactions, kinetic energy, potential energy), called *Hamiltonian* of the system. By proceeding as before, one obtains the fundamental result of SM that in thermal equilibrium each of the possible states x occurs with a probability

$$p(\boldsymbol{x}) = \frac{1}{Z(\beta)}\, \mathrm{e}^{-\beta\mathcal{H}(\boldsymbol{x})}$$

where the Lagrange multiplier for the average energy E is $\lambda_1 = -\beta = -1/T$. This is known as the *Gibbs-Boltzmann distribution*, i.e. distribution of states at equilibrium for a system at temperature T, when the energy structure of each possible configuration $\boldsymbol{x}$ is described by $\mathcal{H}(\boldsymbol{x})$. The partition function Z thus reads

$$Z(\beta) = \sum_{\boldsymbol{x}} \mathrm{e}^{-\beta\mathcal{H}(\boldsymbol{x})}\,.$$

It is easy to show[1] that the free energy $F = E - TS$ is the Lagrangian of the entropy maximization subject to constraints on the average energy.

2. Stochastic processes

Definition 2.1 (formal). *A stochastic process is defined as a collection of random variables X_t indexed by $t \in T$ with some set T, all taking values in the same sample space Ω, which must be measurable with respect to event space $\mathcal{F}$ and measure $\mathbb{P}$.*

Informally, we can say that $(X_t, t \in T)$ is a stochastic process in probability space $(\Omega, \mathcal{F}, \mathbb{P})$ if for any $t \in T$, the corresponding X_t is a random variable in $(\Omega, \mathcal{F}, \mathbb{P})$. Usually, due to a nature of the process we distinguish

(1) discrete-time processes if T is finite or countable, e.g. $T = \mathbb{Z}$ or $T = \mathbb{N}$;
(2) continuous-time processes, if T is uncountable, e.g. $T = \mathbb{R}$ or $T = \mathbb{R}_+$.

Stationary processes play a very relevant role in the study of stochastic processes.

[1] Do it as exercise.

DEFINITION 2.2. *Let $(X_t, t \in T)$ be a stochastic process and let $\Phi_X(x_{t_1}, \dots, x_{t_k})$ be the cumulative distribution function of the joint distribution of X_t at times $t_1, \dots, t_k$, i.e.,*

$$\Phi_X(x_{t_1}, \dots, x_{t_k}) \coloneqq \mathbb{P}[X_{t_1} < x_{t_1}, \dots, X_{t_N} < x_{t_N}].$$

Then, $(X_t, t \in T)$ is said to be strictly (or strongly) stationary if, for all k, for all τ, and for all $t_1, \dots, t_k$

$$\Phi_X(x_{t_1+\tau}, \dots, x_{t_k+\tau}) = \Phi_X(x_{t_1}, \dots, x_{t_k}).$$

A stochastic process is called *Markov process* if the next value of the process depends on the current value, but it is conditionally independent of the previous values of the stochastic process. More precisely, let $(\Omega, \mathcal{F}, \mathbb{P})$ be a probability space with a filtration $\{\mathcal{F}_s\}_{s \in T}$ for some (totally ordered) index set T: this means that $\forall t \in T$, $\mathcal{F}_t \subseteq \mathcal{F}$ σ-algebra, and if $t < t'$ then $\mathcal{F}_t \subseteq \mathcal{F}_{t'}$. If we have, e.g., a stochastic process $X = \{X_t \colon \Omega \to \mathbb{R}\}_t$, we say that the process is *adapted* to such filtration if X_s is measurable on $\mathcal{F}_s$: in a sense, the process "cannot see in the future".

☞ Suppose for example that we consider the process X_t given by two coin tosses, with $t = 1, 2$. Denoting $\Omega_0 = \{H, T\}$ as the space of outcome of one coin toss, the space of possible outcomes is

$$\Omega = \Omega_0 \times \Omega_0.$$

At time $t = 0$ we have that

$$\mathcal{F}_0 = \{\emptyset, \Omega\}$$

because we have no information: there are two possible events, something happens, Ω, with probability 1, and nothing happens, $\emptyset$, with probability zero. Then we toss a coin. Now we have

$$\mathcal{F}_1 = \{\emptyset, \Omega, \{H\} \times \Omega_0, \{T\} \times \Omega_0\}$$

Indeed, we know what the outcome of the first toss was, so we added to our sets options with given first element, but all elements in $\mathcal{F}_1$ have no information about the second toss. After the second toss, we can add as events the specific detailed sequences of outcomes, i.e.,

$$\mathcal{F}_2 = \{\emptyset, \Omega, \{H\} \times \Omega_0, \{T\} \times \Omega_0, \{H, T\}, \{H, H\}, \{T, H\}, \{T, T\}\}$$

which are all subsets of Ω. The sequence $\mathcal{F}_0 \subseteq \mathcal{F}_1 \subseteq \mathcal{F}_2$ is a filtration.

The stochastic process is said to satisfy the *Markov property* if, for each $A \subseteq \mathbb{R}$ and each $s, t \in T$ with $s < t$,

$$\mathbb{P}[X_t \in A | \mathcal{F}_s] = \mathbb{P}[X_t \in A | X_s].$$

In the case in which $T = \mathbb{N}$, given a sequence $\{A_n\}_n$, this can be reformulated as follows:

$$\mathbb{P}[X_n \in A_n | X_{n-1} \in A_{n-1}, \dots, X_0 \in A_0] = \mathbb{P}[X_n \in A_n | X_{n-1} \in A_{n-1}].$$

EXAMPLE [Random walk on $\mathbb{Z}$] Let us assume that we have a particle moving along the $\mathbb{Z}$ lattice according to the following dynamics: starting from $X_0 = 0$, every second it chooses to jump to the right with probability $p \in (0, 1)$ and to the left with probability $1 - p$. We denote X_t the position of the particle at time t Obviously, its position at time

$t = n$ depends only on a position at time $t = n - 1$. This process is not stationary, but it is Markovian. The process is called symmetric if $p = 1/2$. Let us mention that all variables $X_{m+1} - X_m$ are independent and have mean $2p - 1$ and variance 1, so that

$$\mathbb{E}[X_n] = \mathbb{E}[X_n - X_{n-1} + X_{n-1} - X_{n-2} + \ldots + X_1 - X_0] = n(2p-1).$$

And one can see that for a symmetric random walk average displacement is 0. Let $m \geq n$, then

$$\mathbb{E}[X_n X_m] = \mathbb{E}[X_n^2] + \mathbb{E}[X_n (X_m - X_n)] = \mathbb{E}[X_n^2] + \mathbb{E}[X_n]\mathbb{E}[X_{m-n}],$$

where we used statistical independence of $X_m - X_n$ and X_n and the observation that the difference $X_m - X_n$ is distributed as X_{m-n}. Moreover,

$$\begin{aligned}\mathbb{E}[X_n^2] &= \mathbb{E}[(X_n - X_{n-1} + X_{n-1} - X_{n-2} + \ldots + X_1 - X_0)^2] \\ &= \mathbb{E}[(X_n - X_{n-1})^2 + \ldots + (X_1 - X_0)^2 + 2\sum_{j<k} (X_{n-j} - X_{n-j-1})(X_{n-k} - X_{n-k-1})] \\ &= n + n(n-1)(2p-1)^2.\end{aligned}$$

Finally

$$\mathrm{Cov}[X_n, X_m] = n\left(4p - 4p^2\right) = 4p(1-p)\min\{n, m\}.$$

Continuous Markovian processes satisfy the following

THEOREM 2.1 (Chapman-Kolmogorov equation). *For any $s < \tau < t \in T$ and $x, y \in S$*

$$\rho(x, t|y, s) = \int \rho(x, t|z, \tau)\, \rho(z, \tau|y, s)\, \mathrm{d}\, z.$$

Finally, a relevant type of Markov processes are Markov chains.

DEFINITION 2.3. *A Markov chain is a type of Markov process that has either discrete state space or discrete index set (often representing time).*

EXAMPLE [Wiener process/Brownian motion] The Wiener process $(W_t, t \in \mathbb{R}_+)$ is characterised by the following properties:

(1) $W_0 = 0$ almost surely;
(2) W_t has independent increments, i.e., for $\forall t > 0$, the future increments $W_{t+u} - W_t$, for $u \geq 0$, are independent of the past values $\{W_s, s \leq t\}$.
(3) W_t has Gaussian increments, i.e. $W_{t+u} - W_t$ is normally distributed with mean 0 and variance u : $W_{t+u} - W_t \sim \mathcal{N}(0, u)$.
(4) W_t is continuous in t almost surely.

We calculate below expectation and covariance of the values of Wiener process at different times.

$$\mathbb{E}[W_t] = \mathbb{E}[W_t - W_0 + W_0] = \mathbb{E}[W_t - W_0] + \mathbb{E}[W_0] = 0.$$

Let $t \geq s$, then

$$\begin{aligned}\mathbb{E}[W_t W_s] &= \mathbb{E}[(W_t - W_s) W_s + W_s^2] = \mathbb{E}[W_t - W_s]\mathbb{E}[W_s] + \mathbb{E}[W_s^2] \\ &= \mathbb{E}[W_s^2] = \mathbb{E}[(W_s - W_0)^2 + 2(W_s - W_0) W_0 + W_0^2] = s.\end{aligned}$$

And finally

$$\mathrm{Cov}[W_t, W_s] = \min\{t, s\}.$$

Brownian motion can be thought as a limit of simple symmetric random walk with diffusional scaling.

3. Path integration

Gaussian integrals are the basic tools behind the *functional integral* formalism (or *path* integral), which has prominent relevance in modern physics and mathematics. Suppose that we have a walker on a real line starting in x_0 at $n = 0$, so $p_0(x) = \delta(x - x_0)$. This walker is subject to a Markovian dynamics: at each time $n = 1, 2, \dots$, it jumps to a new position with some probability. The probability of the particle of being in position x at step n is equal to

$$p_t(x_n) = \int \mathrm{d}\, x_{n-1} \rho(x_n, x_{n-1}) p_{n-1}(x_{n-1}), \qquad \int \mathrm{d}\, x_n \rho(x, x') = 1,$$

where $\rho(x, x')$ is the probability to jump from x' to x: here we are assuming that the process is homogenous, i.e., q does not depend on time. We also assume that the process is translational invariant, e.g., $\rho(x, x') \equiv \rho(x - x')$ so that $\rho(r)$ decays reasonably fast for large $|r|$. Due to the Markov process we can write

$$\begin{aligned} p_n(x_n) &= \int \mathrm{d}\, x_{n-1}\, \rho(x_n - x_{n-1}) p_{n-1}(x_{n-1}) \\ &= \int \mathrm{d}\, x_{n-1} \int \mathrm{d}\, x_{n-2}\, \rho(x_n - x_{n-1}) \rho(x_{n-1} - x_{n-2}) p_{n-2}(x_{n-2}) \\ &= \prod_{k=1}^{n-1} \left[\int \mathrm{d}\, x_k \rho(x_k - x_{k-1}) \right]. \end{aligned}$$

If we choose

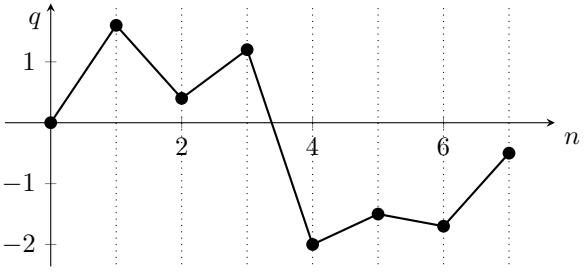
$$\rho(r) = \frac{1}{\sqrt{2\pi\sigma^2}}\, \mathrm{e}^{-\frac{r^2}{2\sigma^2}}$$

then the integral can be written as

$$p_n(x_n) = \frac{1}{(2\pi\sigma^2)^{\frac{n-1}{2}}} \prod_{k=1}^{n-1} \left[\int \mathrm{d}\, x_k \right] \mathrm{e}^{-\mathcal{S}(\boldsymbol{x})}$$

where $\boldsymbol{x} = (x_0, \dots, x_n)$ and

$$\mathcal{S}(\boldsymbol{x}) \coloneqq \sum_{k=0}^{n-1} \frac{(x_k - x_{k-1})^2}{2\sigma^2}$$



Let us now introduce a 'time' variable

$$t_k = k\epsilon, \qquad k = 0, \dots, n, \qquad t_n = n\epsilon \equiv t$$

and the new variable

$$q(\tau)=\sqrt{\epsilon}\left[x_{k-1}+\frac{\tau-t_{k-1}}{\epsilon}(x_k-x_{k-1})\right] \text{ for } t_{k-1}<\tau<t_k, \qquad \begin{cases} q(0)=\sqrt{\epsilon}x_0\equiv q_i, \\ q(t_k)=\sqrt{\epsilon}x_k \\ q(t)=\sqrt{\epsilon}x_n\equiv q_f, \end{cases}$$

With this change of variable for $\tau \neq \epsilon, 2\epsilon, 3\epsilon, \dots$

$$\left.\frac{\mathrm{d}\, q(\tau)}{\mathrm{d}\,\tau}\right|_{\tau\in(t_{k-1},t_k)} = \frac{x_k - x_{k-1}}{\epsilon}.$$

As a result

$$\mathcal{S}(\boldsymbol{x}) = \frac{\epsilon}{2\sigma^2}\sum_{k=0}^{n-1}\left(\left.\frac{\mathrm{d}\, q(\tau)}{\mathrm{d}\,\tau}\right|_{\tau\in(t_{k-1},t_k)}\right)^2 \xrightarrow{\epsilon\to 0} \frac{1}{2\sigma^2}\int_0^t \dot{q}^2(\tau)\,\mathrm{d}\,\tau \equiv \mathcal{S}[q(t)]$$

We have transformed now the argument of the exponent in a *functional* depending on the function $q(t)$. The integral has to be performed on all possible functions $q(t)$ and we formally write

$$\prod_{k=1}^{n-1}\left[\int \mathrm{d}\, x_k\right] \xrightarrow{\epsilon\to 0} \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q(t)]$$

and our integral becomes

$$\mathcal{Z}[q_f|q_i] = \int_{q(0)=q_i}^{q(t)=q_f} \mathcal{D}[q(t)]\,\mathrm{e}^{-\mathcal{S}[q(t)]}$$

This is a general structure that appears when studying measures over paths. In particular, integrals take the form

$$\mathcal{Z}[\boldsymbol{q}_f|\boldsymbol{q}_i] = \int_{\boldsymbol{q}(0)=\boldsymbol{q}_i}^{\boldsymbol{q}(t)=\boldsymbol{q}_f} \mathcal{D}[\boldsymbol{q}(t)]\ \mathrm{e}^{-\mathcal{S}[\boldsymbol{q}(t)]}$$

where $S[\boldsymbol{q}]$ is called *action* of the system. The notion of action is descends from the *Lagrangian formalism* and it is defined as

$$\mathcal{S}[\boldsymbol{q}(t)] = \int_0^t \mathcal{L}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t))\,\mathrm{d}\, t$$

where the argument of the integration $\mathcal{L}(\boldsymbol{q}(t), \dot{\boldsymbol{q}}(t))$ is the *Lagrangian* of the system, in general a function of $\boldsymbol{q}(t)$ and its time derivatives that contains information on the dynamics of the system: in the case of the walker described above, the Lagrangian was $\mathcal{L}(\dot{q}(t)) = \frac{\dot{q}^2}{2\sigma^2}$. As $\mathcal{S}[\boldsymbol{q}(t)]$ is a *functional*, the integration over $\boldsymbol{q}(t)$ is referred to as *functional integration*: $\mathcal{D}[\boldsymbol{q}(t)]$ is meant as the integration over all space of functions $\boldsymbol{q}(t)$. $\mathcal{D}[\boldsymbol{q}(t)]$ is just a formal notation, as more precisely this integration must be intended with a discretized time, in order to retrieve the analogy with ordinary integration, thus a continuous trajectory of evolution $x_i(t)$ must thought as given by a series of points each one corresponding to a discrete time step: the final results are then transformed again into continuous time. Path integrals are

an alternative formulation of Statistical Mechanics that turn out to be particularly convenient for some calculations in dynamical problems.

As a counterpart of functional integration, one can define a *functional derivation*

$$\frac{\delta \mathcal{S}[q(t)]}{\delta q(\tau)}$$

that gives the infinitesimal variation of $\mathcal{S}$ that follows from an infinitesimal variation of the trajectory $q(t) \to q(t) + \delta q$ at time τ. To be more precise, the functional derivative of $\mathcal{S}$ is defined via an integral, i.e., given an arbitrary function $\phi(t)$, $\frac{\delta \mathcal{S}[q(t)]}{\delta q(\tau)}$ is the function such that

$$\int \frac{\delta \mathcal{S}[q(t)]}{\delta q(\tau)} \phi(\tau)\, \mathrm{d}\,\tau = \lim_{\epsilon \to 0} \frac{\mathcal{S}[q(t) + \epsilon\phi(t)] - \mathcal{S}[q(t)]}{\epsilon} \equiv \left. \frac{\mathrm{d}\, \mathcal{S}[q(t) + \epsilon\phi(t)]}{\mathrm{d}\,\epsilon} \right|_{\epsilon=0}$$

It is easy to check that this implies that, if for example $\mathcal{S}[q(t)] = q(t)$, then

$$\frac{\delta q(t)}{\delta q(\tau)} = \delta(t - \tau).$$

Similarly, $\frac{\delta q^n(t)}{\delta q(\tau)} = n q^{n-1}(\tau)\delta(t-\tau)$, and so on. Finally, if $\mathcal{S}[q(t)] = \int_0^t q^\alpha(\tau)\, \mathrm{d}\,\tau$, then

$$\frac{\delta \mathcal{S}[q(t)]}{\delta q(\tau)} = \int_0^t \frac{\delta q^\alpha(t')}{\delta q(\tau)}\, \mathrm{d}\, t' = \alpha \int_0^t q^{\alpha-1}(t')\delta(t'-\tau)\, \mathrm{d}\, t' = \alpha q^{\alpha-1}(\tau).$$

The *principle of least action* states that the classical trajectory is the one that makes the action stationary, i.e., the trajectory solving the equation

$$\frac{\delta \mathcal{S}[\boldsymbol{q}(t)]}{\delta \boldsymbol{q}(\tau)} = 0.$$

This is equivalent to say that the classical trajectory is the one that gives the largest contribution to the partition function $\mathcal{Z}$

As the partition function can be expressed as a path integral, so do the n-points correlation functions,

$$\mathbb{E}[q(t_1)\dots q(t_n)] = \frac{1}{\mathcal{Z}} \int \mathcal{D}[q(t)] q(t_1)\dots q(t_n)\, \mathrm{e}^{-\mathcal{S}[q(t)]}$$

In analogy with moment generating function one can introduce *moment generating functionals*

$$\mathcal{Z}[J] = \int \mathcal{D}[q(t)]\, \mathrm{e}^{-\mathcal{S}[q(t)] + \int_0^t J(\tau) q(\tau)\, \mathrm{d}\,\tau}$$

that generates all the moments by functional derivation

$$\mathbb{E}[q(t_1)\dots q(t_n)] = \frac{1}{\mathcal{Z}[J]} \frac{\delta}{\delta J(t_1)} \cdots \frac{\delta}{\delta J(t_n)} \mathcal{Z}[J] \Big|_{J=0}$$

Exercises

(1) The Wiener-Lévy process was originally introduced to describe the behaviour of the position of a free Brownian particle in one dimension. On the other hand, it plays a central role in the rigorous foundation of the

stochastic differential equations and occurs often in applied mathematics, physics and economics. The Wiener-Lévy process is defined through

$$P_{1|1}\left(x_2,t_2|x_1,t_1\right)=\frac{1}{\sqrt{2\pi\left(t_2-t_1\right)}}\exp\left\{-\frac{\left(x_1-x_2\right)^2}{2\left(t_2-t_1\right)}\right\}.$$

with $t_2>t_1>0$ and condition $P_1\left(x_1,0\right)=\delta(x_1)$.

(a) Show that the probability density for $t_1>0$ is

$$P_1\left(x_1,t_1\right)=\frac{1}{\sqrt{2\pi t_1}}\exp\left(-\frac{x_1^2}{2t_1}\right),$$

and prove that $P_1(x,t)$ satisfies the diffusion equation

$$\frac{\partial P_1(x,t)}{\partial t}=\frac{1}{2}\frac{\partial^2 P_1(x,t)}{\partial x^2}.$$

This is a non-stationary.

(b) Show that

$$\left\langle x\left(t_1\right)\right\rangle=0,\qquad \left\langle x\left(t_1\right)x\left(t_2\right)\right\rangle=\min\left(t_1,t_2\right).$$

(2) The Ornstein-Uhlenbeck (OU) process was constructed to describe the behaviour of the velocity of a free Brownian particle in one dimension. It also describes the position of an over damped particle in a harmonic potential. It is defined by ($\tau>0$)

$$P_1(x)=\frac{1}{\sqrt{2\pi}}\exp\left(-\frac{x^2}{2}\right),$$

$$P_{1|1}\left(x_2,t+\tau|x_1,t\right)=\frac{1}{\sqrt{2\pi\left(1-\mathrm{e}^{-2\tau}\right)}}\exp\left\{-\frac{\left(x_2-x_1\,\mathrm{e}^{-\tau}\right)^2}{2\left(1-\mathrm{e}^{-2\tau}\right)}\right\}.$$

The OU process is stationary, Gaussian and Markovian. According to Doob's theorem, it is essentially the only process with these three properties.

(a) The Gaussian property is clear for P_1. By using $P_2\left(x_2,t_2;x_1t_1\right)=P_1(x_1)P_{1|1}\left(x_2,t_2|x_1,t_1\right)$ show that $P_2\left(x_2,t_2;x_1t_1\right)$ can be identified with a bivariate Gaussian distribution.

(3) Show that the OU process has an exponential autocorrelation function

$$\left\langle x\left(t+\tau\right)x\left(t\right)\right\rangle=\mathrm{e}^{-\tau}.$$

The evolution with time of the velocity correlation has a clear meaning. For short time differences the velocity of the Brownian particle is strongly correlated with itself. As time elapses, the velocity looses all memory of its value at the initial time due to the collisions and hence $P_2\left(x_2,t_2;x_1t_1\right)$ is completely uncorrelated.

(4) Explain why the Chapman-Kolmogorov equation does not hold for non-Markovian processes.

(5) Calculate KL divergence between the distributions of possible outcomes for M throws of fair (probability of head is $1/2$) and unfair (probability of head is $1/3$) coins.

LECTURE 6

Methods for ODEs and PDEs

In this chapter we will discuss some methods for the solution of ordinary differential equations (ODEs). To do so, we will first start reviewing some results about *dynamical systems*, and then solve the associated differential equations. In the second part of the lecture we will give a brief introduction to PDEs and their classification, and we will discuss some methods of solving them.

1. Dynamical systems

Dynamical systems (DS) are systems described by a n-dimensional, time dependent vector $\boldsymbol{x}(t)$, governed by dynamical laws given in terms of an ODE in the form

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, t)$$

The function $\boldsymbol{f}$ is a *velocity field* for the dynamical system. The dynamical system is also said to be of *order* n. If time t does not explicitly appear in the velocity function $\boldsymbol{f}$, the system is said to be *autonomous*, otherwise it is *non-autonomous*. Thus for autonomous systems, we have $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x})$. Note that every non-autonomous DS can be considered as an autonomous one, by introducing new "coordinate" s such that the resulting DS is of order $n+1$ with $\frac{\mathrm{d}\, t}{\mathrm{d}\, s} = 1$.

Definition 1.1. *The set of points* $\{\boldsymbol{x}(t), t \in \mathbb{R}\}$ *which solve* $\dot{\boldsymbol{x}} = \boldsymbol{f}(\boldsymbol{x}, t)$*, and for which* $\boldsymbol{x}(t_0) = \boldsymbol{x}_0$ *is called the orbit of the DS passing through* $\boldsymbol{x}_0$*. The set of all orbits obtained by varying* t_0 *and* $\boldsymbol{x}_0$ *through all physically allowed values is called the phase-flow of the DS.*

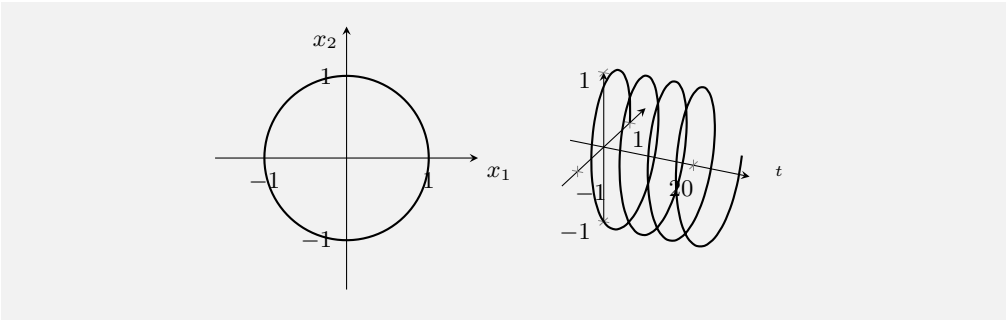
Definition 1.2. *The set of pairs* $(t, \boldsymbol{x}(t))_t$ *which solve the ODEs, and for which* $\boldsymbol{x}(t_0) = \boldsymbol{x}_0$ *is called the trajectory or solution curve of the DS passing through* $\boldsymbol{x}_0$*. The set of all trajectories obtained by varying* t_0 *and* $\boldsymbol{x}_0$ *through all physically allowed values is called the flow of the DS.*

Note the difference between phase-flow and flow; the latter contains more dynamical information than the former.

Example Suppose that we have the dynamical system for $\boldsymbol{x} \in \mathbb{R}^2$

$$\dot{\boldsymbol{x}} = \boldsymbol{f}(t), \qquad \boldsymbol{f}(t) = \begin{pmatrix} -\sin t \\ \cos t \end{pmatrix}, \qquad \boldsymbol{x}(0) = \begin{pmatrix} 1 \\ 0 \end{pmatrix} \Rightarrow \boldsymbol{x}(t) = \begin{pmatrix} \cos t \\ \sin t \end{pmatrix}.$$

Then we can draw the orbit (on the left) and the trajectory (on the right):



DEFINITION 1.3. *A graphical representation of the the phase space, including a graph of the velocity function* $\boldsymbol{f}$ *and a graph of the phase flow, including velocity information, i.e., with* $\boldsymbol{f}(\boldsymbol{x})$ *drawn at representative points* $\boldsymbol{x}$ *in phase space, is called phase portrait of the system (also referred to as phase diagram). The vector* $\boldsymbol{f}(\boldsymbol{x})$ *is called velocity of the flow (at* $\boldsymbol{x}$*).*

DEFINITION 1.4. *A point* $\boldsymbol{a}$ *is called a fixed point of an autonomous DS if*

$$\boldsymbol{f}(\boldsymbol{a}) = \mathbf{0}.$$

A system which is at a fixed point will stay there forever, unless perturbed.

DEFINITION 1.5. *Let* $\boldsymbol{a}$ *be a fixed point of a DS*

- *A fixed point* $\boldsymbol{a}$ *of a DS is called strongly stable, if all trajectories starting (sufficiently) close to* $\boldsymbol{a}$ *will approach* $\boldsymbol{a}$ *under the dynamics.*
- *A fixed point* $\boldsymbol{a}$ *of a DS is called unstable, if there exist trajectories starting close to* $\boldsymbol{a}$ *which will evolve away from* $\boldsymbol{a}$ *under the dynamics. (Note that in n-th order DS, mixed situations exist, i.e. some subset of the trajectories starting sufficiently close to* $\boldsymbol{a}$ *will approach* $\boldsymbol{a}$*, whereas there exist others which will evolve away from* $\boldsymbol{a}$*, no matter how close to* $\boldsymbol{a}$ *they start.)*
- *A fixed point* $\boldsymbol{a}$ *of a DS is called (marginally) stable, if all trajectories starting (sufficiently) close to* $\boldsymbol{a}$ *will neither approach* $\boldsymbol{a}$ *under the dynamics, nor will they evolve away from it, but rather 'keep circling around'.*

1.1. Connection to nth order ODE. The general nth order differential equation has the form

$$F\left(\partial_t^n x(t), \partial_t^{n-1} x(t), \ldots, \partial_t x(t), x(t), t\right) = 0,$$

for some function $F : \mathbb{R}^{n+2} \to \mathbb{R}$. Assume that this can be can be rewritten as

$$\partial_t^n x(t) = G\left(\partial_t^{n-1} x(t), \ldots, \partial_t x(t), x(t), t\right),$$

for some function $G : \mathbb{R}^{n+1} \to \mathbb{R}$. Then introducing $\boldsymbol{y}(t) \in \mathbb{R}^n$ we can write an equivalent nth order DS

$$\begin{cases} \dot{y}_1 &= y_2, \\ \dot{y}_2 &= y_3, \\ \vdots & \\ \dot{y}_n &= G\left(y_n, y_{n-1}, \ldots, y_1, t\right). \end{cases}$$

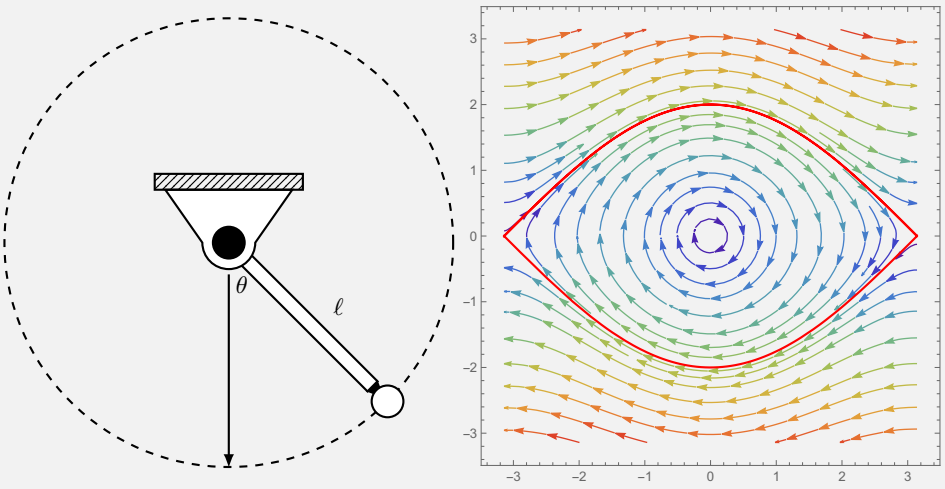
A valuable tool for the study of first order DS is the so-called *phase portrait*. It is a geometric representation of the trajectories in the *phase space*, i.e., the space of all

systems configurations. In the phase portrait, each curve corresponds to an initial condition. They immediately provide evidences of the presence of *attractors* (i.e., stable points), *repellors* (i.e., unstable points) or *limit cycles*.

EXAMPLE The simple pendulum satisfies the following equation

$$\ddot{\theta} = -\frac{g}{\ell}\sin\theta \Leftrightarrow \begin{cases} \dot{y}_1 &= y_2, \\ \dot{y}_2 &= -\frac{g}{\ell}\sin y_1. \end{cases}$$

The system is therefore described by a two dimensional vector $\boldsymbol{y} \in \mathbb{R}^2$, such that $y_1 = \theta$ and $y_2 = \dot{\theta}$: its phase portrait is a 2-dimensional diagram, where each curve corresponds to a given initial condition. It appears clearly that $\theta = \dot{\theta} = 0$ is a stable point, $\theta = \pm\pi$ with $\dot{\theta} = 0$ are unstable points, and there are no limit cycles (i.e., cycles attracting nearby trajectories for $t \to +\infty$).



1.2. First Order DS. A first order autonomous dynamical system is described by a differential equation of the form

$$\frac{\mathrm{d}\,x}{\mathrm{d}\,t} = f(x), \quad x \in \mathbb{R} \qquad f : \mathbb{R} \to \mathbb{R}$$

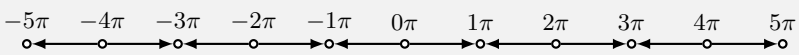
If we want to solve for the evolution of the system, it depends solely on the initial value x of the state variable describing the system under consideration. The phase space is given by the set of admissible values for x. For example, if x is the chemical concentration of a substance, the allowed values of x are such that $x > 0$.

Phase portrait can now be thought as a plot of $f(x)$, plot of corresponding vector field on X-axis and a plot of phase flow. It is also of a big importance to distinguish regions of positivity and negativity of $f(x)$. This is clearly seen from the following observation: if $f(x) > 0$, then x increases as function of t, while if $f(x) < 0$ then x decreases as function of t.

EXAMPLE Let us consider DS defined by

$$\dot{x} = \sin x.$$

Then the phase space is just the real line:



One can see that there are infinitely many stationary points given by $a_k = \pi k$, $k \in \mathbb{Z}$. The dynamics tries to push the particle out of points a_{2k} towards points a_{2k-1} or a_{2k+1}. This suggests that point a_{2k} are unstable, while a_{2k+1} are stable. The phase space is divided now into regions of positivity for $f(x)$, negativity and stationary points. If initial position $x(0)$ is in the region of positivity, then the particle moves to the right, according to a vector field $v = f(x)$, until it reaches close neighbourhood of a stable point. This stable point will be a barrier for a particle as it can't cross it.

1.2.1. *Linear stability of a fixed point.* Let us focus now on the stability properties of fixed points in first order DS. The stability analysis based on (and requiring only) Taylor series expansions to first order is referred to as *linear stability analysis* of a fixed point. Corresponding fixed points are called *linearly stable or unstable*. If $f(x)$ is suitably differentiable, we can approximate $f(x)$ by its Taylor expansion around a fixed point $x = a$

$$f(x) = f'(a)(x-a) + \frac{f''(a)}{2}(x-a)^2 + \dots \qquad \text{being } f(a) = 0.$$

Let us assume that $f'(a) \neq 0$; then for $|x-a| \ll 1$ one can approximate the differential equation describing the evolution of the system as

$$\dot{x} \simeq f'(a)(x-a) \to \frac{\mathrm{d}(x-a)}{\mathrm{d}\,t} \simeq f'(a)(x-a) \Rightarrow (x-a) \sim (x_0-a)\,\mathrm{e}^{f'(a)t}.$$

Here we have assumed our initial position to be $x_0 \in \dot{\mathcal{B}}\,(a,\varepsilon)$. We can see that

- If $f'(a) > 0$, $|x-a|$ increases exponentially in time and we say that a is a linearly unstable fixed point.
- If $f'(a) < 0$, $|x-a|$ decreases exponentially in time and we say that a is a linearly stable fixed point.

EXAMPLE In the DS $\dot{x} = \sin x$, for a fixed point $a_k = \pi k$ we have $f'\,(a_k) = \cos(\pi k) = (-1)^k$. Therefore, points a_{2k+1} are linearly stable, and a_{2k} are linearly unstable.

Note that the approximate solution of the ODEs describing the DS near fixed points based on Taylor series expansions is valid only in the vicinity of fixed points. The quality of the approximate description will therefore improve, if a fixed point is approached under the dynamics, whereas the approximate description deteriorates, if the system moves away from a fixed point.

1.3. Second Order DS. A second order autonomous dynamical system is described by differential equations of the form

$$\begin{cases} \frac{\mathrm{d}\,x_1}{\mathrm{d}\,t} &= f_1\,(x_1,x_2)\,, \\ \frac{\mathrm{d}\,x_2}{\mathrm{d}\,t} &= f_2\,(x_1,x_2)\,. \end{cases}$$

or in vector form

$$\frac{\mathrm{d}\,\boldsymbol{x}}{\mathrm{d}\,t} = \frac{\mathrm{d}}{\mathrm{d}\,t}\begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \boldsymbol{f}(\boldsymbol{x}) = \begin{pmatrix} f_1(\boldsymbol{x}) \\ f_2(\boldsymbol{x}) \end{pmatrix}.$$

The *phase space* Γ is defined as the set of admissible values for $\boldsymbol{x}$. The pair (x_1, x_2) denotes a point in $\mathbb{R}^2$, so generally $\Gamma \subseteq \mathbb{R}^2$. For some systems, Γ may be a

proper subset of $\mathbb{R}^2$. A point $\boldsymbol{a} \in \mathbb{R}^2$ is a *fixed point* of the dynamical system, iff $f_1(\boldsymbol{a}) = f_2(\boldsymbol{a}) = 0$.

DEFINITION 1.6. *The set of points $\boldsymbol{a} \in \mathbb{R}^2$ for which $f_1(\boldsymbol{a}) = 0$ is called null-cline of f_1. Similarly, the set of points $\boldsymbol{a} \in \mathbb{R}^2$ for which $f_2(\boldsymbol{a}) = 0$ is called null-cline of f_2*

On a null-cline of f_1, the x-component of the velocity vanishes; similarly, on a null-cline of f_2, it is the y-component of the velocity which is zero. Fixed points are intersections of the null-clines of f_1 and f_2. The defining equation of the null-cline, $f_1(\boldsymbol{a}) = 0$ generally defines a curve in $\mathbb{R}^2$.

1.3.1. *Stability of a fixed point.* The stability problem for second order autonomous systems is likely to be more complicated than for first order systems; the extra dimension allows more possibilities.

DEFINITION 1.7. *We say that the fixed point $\boldsymbol{a}$ is an attractor for a particular DS if $\boldsymbol{x}(t) \to \boldsymbol{a}$ as $t \to \infty$. We say that a fixed point $\boldsymbol{a}$ is strongly stable if it is an attractor for all phase curves which enter some neighbourhood of $\boldsymbol{a}$.*

This conveys the notion that all phase curves which pass sufficiently close to $\boldsymbol{a}$ are "sucked in" to $\boldsymbol{a}$ as $t \to \infty$. The following definition provides a weaker concept of stability.

DEFINITION 1.8. *We say that a fixed point $\boldsymbol{a}$ is stable if for every neighbourhood $\mathcal{N}_1$ of $\boldsymbol{a}$ there exists a neighbourhood $\mathcal{N}_2$ of $\boldsymbol{a}$, $\mathcal{N}_2 \subseteq \mathcal{N}_1$, such that $\boldsymbol{x}(0) \in \mathcal{N}_2 \Rightarrow \boldsymbol{x}(t) \in \mathcal{N}_1$ for all $t \geq 0$.*

Roughly speaking this definition says that if $\boldsymbol{a}$ is a stable fixed point then any motion of the system which starts close enough to $\boldsymbol{a}$ remains close to $\boldsymbol{a}$. Notice that this definition does not require that the system tends to $\boldsymbol{a}$ as $t \to \infty$. If $\boldsymbol{a}$ is strongly stable then it is stable, but the converse is not true.

EXAMPLE Let us consider 2nd order DS defined by

$$\begin{cases} \frac{\mathrm{d}\, y_1}{\mathrm{d}\, t} &= y_2, \\ \frac{\mathrm{d}\, y_2}{\mathrm{d}\, t} &= -\sin y_1 \end{cases}$$

corresponding to the simple pendulum, as we already saw. However, we just want to comment its phase portrait at page 77 and analyse it qualitatively. First we find null-clines: for f_1 it is the line $y_2 = \dot{\theta} = 0$, for f_2 there are infinitely many lines $y_1 = \theta = \pi k$. Corresponding fixed points are $\boldsymbol{a}_k = (\pi k, 0)$. From the sketch of vector field we can see that if the particle in the upper half plane, then it moves to the right, until (if this happens) it reaches the null-cline for f_1. If it crosses the null-cline, then it starts to go to the left, and so on. It can also be seen from the picture (and can be analytically calculated), that points $\boldsymbol{a}_k$ are stable (but not strongly stable) for even indexes and unstable otherwise.

1.4. Separable systems. In second order dynamical systems the dynamical evolutions of the variables x_1 and x_2 are quite generally coupled: both velocity functions depend on x_1 and x_2. Sometimes it is possible to change variables from (x_1, x_2) to new variables (y_1, y_2) in such a way that the differential equations describing the system take the form

$$\begin{cases} \dot{y}_1 = v_1(y_1), \\ \dot{y}_2 = v_2(y_2). \end{cases}$$

In this case we say that the system is separable in the variables (y_1, y_2): the second order system has been decoupled into two first order systems described by the first order differential equations $\dot{y}_1 = v_1(y_1)$ and $\dot{y}_2 = v_2(y_2)$ respectively.

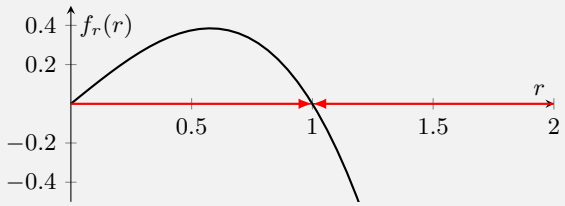
EXAMPLE Let us consider 2nd order DS defined by

$$\begin{cases} \dot{x}_1 = x_1 + x_2 - x_2^3 - x_1 x_2^2, \\ \dot{x}_2 = -x_1 + x_2 - x_1^2 x_2 - x_2^3. \end{cases}$$

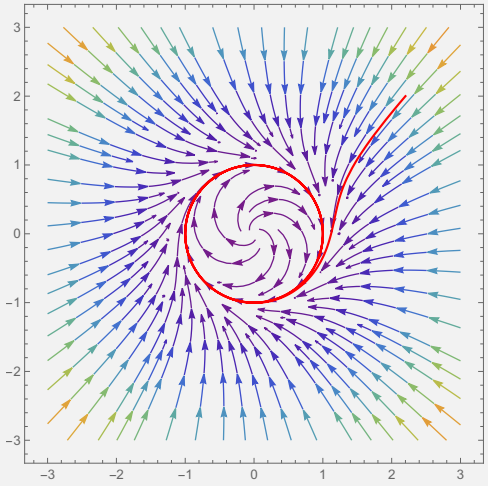
We introduce polar coordinates $(r(t), \theta(t))$ by putting $x_1 = r\cos\theta$ and $x_2 = r\sin\theta$. After some algebraic manipulations,

$$\begin{cases} \dot{r} &= r - r^3, \\ \dot{\theta} &= -1. \end{cases}$$

We managed to transform 2nd order DS to a couple of the first order DS. The second one is simple and means that we are rotating in clockwise direction with constant speed. For the first system we can draw it own phase portrait:



Starting from any positive value of r we end up with $r = 1$ in a limit $t \to \infty$. It can be shown analytically that the system will reach value $r = 1$ in a finite time. After reaching this fixed point r will stay unchanged, while θ will change. And we conclude that our two-dimensional system, starting from any point except the origin, will be "sucked" in a finite time by unit circle, which is a *limit cycle*. After that time the particle will be moving around the origin with period 2π. In the original parametrisation, the phase portrait is the following (in red, a sample trajectory approaching the attractor):



1.5. Linear Second order DS. Unlikely to one-dimensional case, the linear stability analysis in the case of second order DS is less straightforward. Therefore we start first with the linear case and then proceed with the discussion of linear

stability analysis. General form of a linear system is given by

$$\dot{\boldsymbol{x}} = \boldsymbol{A}\boldsymbol{x},$$

where $\boldsymbol{A}$ is a constant matrix. The only fixed point of the system is $\boldsymbol{x} = \mathbf{0}$ and we analyse its stability below. We consider real matrices $\boldsymbol{A}$. Such matrix can *always* be decomposed in a Jordan normal form,

$$\boldsymbol{A} = \mathbf{P}\boldsymbol{J}\mathbf{P}^{-1}, \qquad \boldsymbol{J} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} \quad \text{or} \quad \boldsymbol{J} = \begin{pmatrix} \lambda & 1 \\ 0 & \lambda \end{pmatrix}$$

with $\mathbf{P}$ invertible matrix. Therefore there are two possible cases (we suppose that we impose $\boldsymbol{x}(0) = \boldsymbol{x}_0$):

(1) Let us consider the first case, $\boldsymbol{J} = \left(\begin{smallmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{smallmatrix}\right)$. If $\boldsymbol{A}$ *has two distinct real eigenvalues* $\lambda_1 < \lambda_2$, then there also exist two linearly independent eigenvectors $\boldsymbol{v}_1$ and $\boldsymbol{v}_2$ corresponding to λ_1 and λ_2 respectively, and the general solution of the system is given by

$$\boldsymbol{x}(t) = C_1\,\mathrm{e}^{\lambda_1 t}\,\boldsymbol{v}_1 + C_2\,\mathrm{e}^{\lambda_2 t}\,\boldsymbol{v}_2,$$

where C_1, C_2 are some constants to be determined by initial conditions $\boldsymbol{x}(0) = C_1\boldsymbol{v}_1 + C_2\boldsymbol{v}_2 = \boldsymbol{x}_0$. One can now see that

- if $\lambda_1 < \lambda_2 < 0$, then $\boldsymbol{x}(t) \to \mathbf{0}$ as $t \to \infty$, and $\mathbf{0}$ is a strongly stable point.
- if $\lambda_2 = 0$, then $\boldsymbol{x}(t) \to C_2\boldsymbol{v}_2$, as $t \to \infty$. C_2 is bounded by $C\|\boldsymbol{x}_0\|$, for some constant C. And therefore, $\mathbf{0}$ is a stable fixed point, because $\|\boldsymbol{x}(t)\| \le C\|\boldsymbol{v}_2\|\|\boldsymbol{x}_0\|$.
- if $\lambda_2 > 0$, then $\boldsymbol{x}(t) \to \infty$ and point $\mathbf{0}$ is unstable.

If $\lambda_1 = \lambda_2 = \lambda$, $\boldsymbol{A}$ *is diagonal with* λ*s on a diagonal,* being $\boldsymbol{A} = \lambda\mathbf{P}\boldsymbol{I}_2\mathbf{P}^{-1} = \lambda\boldsymbol{I}_2$. Then solution is given by

$$\boldsymbol{x}(t) = \mathrm{e}^{\lambda t}\,\boldsymbol{u},$$

for some constant vector $\boldsymbol{u}$. And

- $\mathbf{0}$ is a strongly stable fixed point if $\lambda < 0$.
- $\mathbf{0}$ is a stable fixed point if $\lambda = 0$.
- $\mathbf{0}$ is an unstable fixed point if $\lambda > 0$.

(2) Let us consider the second case, $\boldsymbol{J} = \left(\begin{smallmatrix} \lambda & 1 \\ 0 & \lambda \end{smallmatrix}\right)$. Then $\boldsymbol{A}$ *has eigenvalues* $\lambda_\pm = \mu \pm i\nu$ with μ, ν real. It also exists a complex eigenvector $\boldsymbol{v}$ corresponding to λ_+ (with $\overline{\boldsymbol{v}}$ corresponding to λ_-) and the general solution of the system is given by

$$\boldsymbol{x}(t) = \begin{cases} \mathrm{e}^{\mu t}\left(C_1\,\mathrm{e}^{i\nu t}\,\boldsymbol{v} + C_2\,\mathrm{e}^{-i\nu t}\,\overline{\boldsymbol{v}}\right), & \text{if } \nu \neq 0 \\ \mathrm{e}^{\mu t}\left(C_1 + C_2 t\right)\boldsymbol{v}, & \text{if } \nu = 0, \end{cases}$$

where C_1 and C_2 are determined by initial conditions. One can now see that

- if $\mu < 0$, then $\boldsymbol{x}(t) \to \mathbf{0}$ as $t \to \infty$, and $\mathbf{0}$ is a strongly stable point.
- if $\mu = 0$, then the particle moves along the elliptic orbit around the origin and therefore, $\mathbf{0}$ is a stable fixed point, sometimes called *elliptic fixed point.*
- if $\mu > 0$, then $\boldsymbol{x}(t) \to \infty$ and point $\mathbf{0}$ is unstable.

1.6. Linear stability analysis for the second order DS. Given a fixed point $\boldsymbol{a}$, we want to investigate the stability of a fixed point by first Taylor-expanding about $\boldsymbol{a}$

$$f_1(\boldsymbol{x}) = f_1(\boldsymbol{a}) + \frac{\partial f_1(\boldsymbol{a})}{\partial x_1}(x_1 - a_1) + \frac{\partial f_1(\boldsymbol{a})}{\partial x_2}(x_2 - a_2) + o\left(\|\boldsymbol{x} - \boldsymbol{a}\|^2\right),$$
$$f_2(\boldsymbol{x}) = f_2(\boldsymbol{a}) + \frac{\partial f_2(\boldsymbol{a})}{\partial x_1}(x_1 - a_1) + \frac{\partial f_2(\boldsymbol{a})}{\partial x_2}(x_2 - a_2) + o\left(\|\boldsymbol{x} - \boldsymbol{a}\|^2\right).$$

Thus, to the first order in $\|\boldsymbol{x} - \boldsymbol{a}\|$ one can approximate DS in this vectorial form

$$\frac{\mathrm{d}}{\mathrm{d}\,t}(\boldsymbol{x} - \boldsymbol{a}) = \boldsymbol{J_f}(\boldsymbol{x} - \boldsymbol{a}),$$

where $\boldsymbol{J_f}$ is the Jacobian matrix of the system about $\boldsymbol{a}$ (note that the partial derivatives are evaluated at $\boldsymbol{x} = \boldsymbol{a}$) and given by

$$\boldsymbol{J_f} = \begin{pmatrix} \frac{\partial f_1}{\partial x_1} & \frac{\partial f_1}{\partial x_2} \\ \frac{\partial f_2}{\partial x_1} & \frac{\partial f_2}{\partial x_2} \end{pmatrix}.$$

Linear stability can now be analysed using linear model discussed above. As we have already seen in the linear models, stability is determined by the eigenvalues of $\boldsymbol{J_f}$. They are given by

$$\lambda_\pm = \frac{\operatorname{tr} \boldsymbol{J_f} \pm \sqrt{\operatorname{tr}^2 \boldsymbol{J_f} - 4 \det \boldsymbol{J_f}}}{2}.$$

EXAMPLE Let us consider DS defined by

$$\begin{cases} \frac{\mathrm{d}\,x_1}{\mathrm{d}\,t} &= x_2 - x_1^2 + 2, \\ \frac{\mathrm{d}\,x_2}{\mathrm{d}\,t} &= 2\left(x_1^2 - x_2^2\right). \end{cases}$$

and study linear stability for its fixed points. Fixed points are found by solving

$$\begin{cases} x_2 - x_1^2 + 2 &= 0, \\ x_1^2 - x_2^2 &= 0. \end{cases}$$

There are four of them $\boldsymbol{a}_1 = (2,2)$, $\boldsymbol{a}_2 = (-2,2)$, $\boldsymbol{a}_3 = (1,-1)$, $\boldsymbol{a}_4 = (-1,-1)$. The Jacobian of DS is given by

$$\boldsymbol{J} = \begin{pmatrix} -2x & 1 \\ 4x & -4y \end{pmatrix}.$$

(1) Fixed point $\boldsymbol{a}_1$ is linearly stable as we have

$$\boldsymbol{J} = \begin{pmatrix} -4 & 1 \\ 8 & -8 \end{pmatrix}, \quad \lambda_\pm = -6 \pm 2\sqrt{3} < 0.$$

(2) Fixed point $\boldsymbol{a}_2$ is linearly unstable as we have

$$\boldsymbol{J} = \begin{pmatrix} 4 & 1 \\ -8 & -8 \end{pmatrix}, \quad \lambda_- = -2 - 2\sqrt{7} < 0 \text{ and } \lambda_+ = -2 + 2\sqrt{7} > 0.$$

(3) Fixed point $\boldsymbol{a}_3$ is linearly unstable as we have

$$\boldsymbol{J} = \begin{pmatrix} -2 & 1 \\ 4 & 4 \end{pmatrix}, \quad \lambda_1 = 1 - \sqrt{13} < 0 \text{ and } \lambda_2 = 1 + \sqrt{13} > 0.$$

(4) Fixed point $\boldsymbol{a}_4$ is linearly unstable as we have

$$\boldsymbol{J} = \begin{pmatrix} 2 & 1 \\ -4 & 4 \end{pmatrix}, \quad \lambda_1 = 3 - i\sqrt{3} \text{ and } \lambda_2 = 3 - i\sqrt{3}, \quad \text{with} \quad \Re\lambda_1 > 0.$$

2. Methods of solving ODEs

In this section we give a short list of ODEs, which can be solved explicitly. Explicit equations are those which can be solved by direct explicit integration; they are of the form

$$\frac{\mathrm{d}\, x}{\mathrm{d}\, t} = f(t),$$

so that the r.h.s. does not depend on the unknown function x; thus explicit first order equations are not strictly ODEs. Integrating w.r.t. time t one obtains

$$x(t) = F(t) + C,$$

with $F(t) + C$ denoting the indefinite integral of the function f. The constant C, may be fixed by inserting an initial condition, giving $x\left(t_0\right) = x_0 = F\left(t_0\right) + C$, hence $C = x_0 - F\left(t_0\right)$, and $x(t) = x_0 + F(t) - F\left(t_0\right)$. Our goal will be to reduce to this form more complicated ODEs.

2.1. First order separable ODE. Equations of the type

$$\frac{\mathrm{d}\, x}{\mathrm{d}\, t} = f(t)g(x),$$

can be integrated formally by separation of variables:

$$\frac{\mathrm{d}\, x}{g(x)} = f(t)\,\mathrm{d}\, t \Rightarrow \int \frac{\mathrm{d}\, x}{g(x)} = \int f(t)\,\mathrm{d}\, t.$$

Denoting the indefinite integrals involved by $G(x) + c_1 = \int \frac{\mathrm{d}\, x}{g(x)}$ and $F(t) + c_2 = \int f(t)\,\mathrm{d}\, t$, combining the two integration constants into one, one obtains

$$G(x) = F(t) + C,$$

which – on (formally) solving for x – gives

$$x = G^{-1}\left(F(t) + C\right),$$

with arbitrary C as the general solution. The constant C can be fixed by inserting an initial condition, giving $C = G\left(x_0\right) - F\left(t_0\right)$.

EXAMPLE Consider the ODE

$$\frac{\mathrm{d}\, x}{\mathrm{d}\, t} = \alpha x,$$

where α is a constant. This equation arises frequently in our work, see e.g., linear approximation for DS. We have

$$\frac{\mathrm{d}\, x}{x} = \mathrm{d}\, t \Rightarrow \ln x = \alpha t + C,$$

and thus

$$x(t) = C\,\mathrm{e}^{\alpha t}.$$

2.2. First order linear ODE. First order, linear equations are of the form

$$\frac{\mathrm{d}\,x(t)}{\mathrm{d}\,t} + f(t)x(t) = g(t), \qquad x(t_0) = x_0,$$

with f and g given functions of t. Equations of this form are solved using the *method of integrating factors*. Let us first solve a homogeneous version with $g(t) = 0$, i.e.

$$\frac{\mathrm{d}\,x_{\mathrm{h}}(t)}{\mathrm{d}\,t} + f(t)x_{\mathrm{h}}(t) = 0.$$

This is solved by separating variables and solution is given by

$$x_{\mathrm{h}}(t) = C\,\mathrm{e}^{-F(t)}, \qquad F(t) = \int_{t_0}^{t} f(s)\,\mathrm{d}\,s,$$

where $F(t)$ is anti-derivative of $f(t)$ and C is a constant. To obtain a solution of non-homogeneous equation we will use the ansatz $x_{\mathrm{ih}}(t) = h(t)\,\mathrm{e}^{-F(t)}$, searching for a proper $h(t)$. Substituting expression for $x_{\mathrm{ih}}(t)$ into original ODE and taking into account properties of $x_{\mathrm{h}}(t)$ we obtain

$$\mathrm{e}^{-F(t)}\,\frac{\mathrm{d}\,h(t)}{\mathrm{d}\,t} = g(t),$$

which can be solved by explicit integration as

$$h(t) = \int g(t)\,\mathrm{e}^{F(t)}\,\mathrm{d}\,t.$$

Combining the above with initial conditions one gets

$$x(t) = x_0\,\mathrm{e}^{-F(t)} + \mathrm{e}^{-F(t)} \int_{t_0}^{t} g\,(\tau)\,\mathrm{e}^{F(\tau)}\,\mathrm{d}\,\tau.$$

EXAMPLE Consider the ODE for $t > 0$

$$t\,(t+1)\,\frac{\mathrm{d}\,x}{\mathrm{d}\,t} - (t+2)\,x = t^3\,(2t-3)\,, \qquad x(1) = x_0.$$

The homogeneous version of the equation reads

$$\frac{\mathrm{d}\,x_{\mathrm{h}}}{x_{\mathrm{h}}} = \frac{(t+2)}{t\,(t+1)},$$

and is solved by

$$\ln x_{\mathrm{h}} = \int \left(\frac{2}{t} - \frac{1}{t+1}\right)\mathrm{d}\,t = \ln\frac{t^2}{t+1} + c_0 \Rightarrow x_{\mathrm{h}}(t) = \frac{Ct^2}{t+1}.$$

Now let $x_{\mathrm{ih}}(t) = \frac{t^2}{t+1}h(t)$, then

$$\frac{t^2}{t+1}\,\frac{\mathrm{d}\,h(t)}{\mathrm{d}\,t} = t^3\,(2t-3)\,.$$

Integrating the last equation we obtain

$$h(t) = \int_{1}^{t} s\,(s+1)\,(2s-3)\,\mathrm{d}\,s = \frac{4}{3} + \frac{1}{2}t^4 - \frac{1}{3}t^3 - \frac{3}{2}t^2,$$

and thus

$$x(t) = \frac{t^2}{t+1}\left(\frac{1}{2}t^4 - \frac{1}{3}t^3 - \frac{3}{2}t^2 + 2x_0\right).$$

2.3. First order homogeneous ODE. Consider the equation

$$\frac{\mathrm{d}\,x}{\mathrm{d}\,t} = \frac{P(t,x)}{Q(t,x)},$$

where P and Q are homogeneous functions of (the same) degree m, meaning that that

$$P(t,\lambda t) = t^m P(1,\lambda) \quad \text{and} \quad Q(t,\lambda t) = t^m Q(1,\lambda),$$

for some m. The general solution of the ODE may be found by making the substitution $x = tv(t)$ where v has to be determined. We have

$$t\frac{\mathrm{d}\,v}{\mathrm{d}\,t} + v = \frac{P(1,v)}{Q(1,v)} \Leftrightarrow t\frac{\mathrm{d}\,v}{\mathrm{d}\,t} = R(v),$$

where $R(v) = \frac{P(1,v)}{Q(1,v)} - v$ and the last equation is an ODE with separable variables and can be solved by using the standard technique.

EXAMPLE Consider the ODE

$$\frac{\mathrm{d}\,x}{\mathrm{d}\,t} = \frac{x^2 - t^2}{2xt}.$$

Changing variables with $x = tv(t)$ one gets

$$t\dot{v} + v = \frac{v^2 - 1}{2v},$$

and after separation of variables we obtain

$$-\frac{2v\,\mathrm{d}\,v}{1+v^2} = \frac{\mathrm{d}\,t}{t}.$$

Integrating last identity we get, for $t > 0$

$$-\ln\left(1+v^2\right) = \ln t + C.$$

A solution for the initial ODE is now given by

$$x^2 + t^2 = Ct,$$

for some constant C.

2.4. Second order linear, with constant coefficients. Second order linear ODEs with constant coefficients are of the form

$$a\frac{\mathrm{d}^2\,x(t)}{\mathrm{d}\,t^2} + b\frac{\mathrm{d}\,x(t)}{\mathrm{d}\,t} + cx(t) = f(t),$$

where a, b, c are constants and $f(t)$ is a given function of time. As before, we will first try to solve homogeneous equation and then using method of varying constants we solve inhomogeneous one.

2.4.1. *The homogeneous case.* We will first consider the special case of homogeneous equations

$$a\frac{\mathrm{d}^2 x(t)}{\mathrm{d}\, t^2} + b\frac{\mathrm{d}\, x(t)}{\mathrm{d}\, t} + cx(t) = 0.$$

Linear and homogeneous ODEs have important properties:

(1) a solution $x(t)$ can be multiplied with an arbitrary constant, and remains a solution;
(2) for any pair x_1 and x_2 of independent solutions (which are not proportional to each other), any linear combination of the solutions x_1 and x_2 with arbitrary constant coefficients is also a solution of the equation

The homogeneous equation is solved with the help of *auxiliary polynomials*. This method is based on the observation that the equation is solved by functions of the form

$$x(t) = \mathrm{e}^{\lambda t},$$

provided λ is properly chosen. The condition on λ is obtained by inserting the exponential ansatz into equation. One gets

$$\left(a\lambda^2 + b\lambda + c\right)\mathrm{e}^{\lambda t} = 0.$$

Since $\mathrm{e}^{\lambda t} \neq 0$, we see that $\mathrm{e}^{\lambda t}$ is a solution of equation provided

$$P(\lambda) = a\lambda^2 + b\lambda + c = 0,$$

which is the auxiliary equation for the auxiliary polynomial P. We consider below only the case of real coefficients (straightforwardly extended to the complex case). The auxiliary equation is a quadratic equation in λ and as such there are three possibilities:

(1) There are two distinct real solutions λ_1, λ_2. It follows that $x_1(t) = \mathrm{e}^{\lambda_1 t}$ and $x_1(t) = \mathrm{e}^{\lambda_1 t}$ are independent solutions of the given differential equation. The general solution of initial homogeneous ODE is now obtained by forming an arbitrary linear combination of these two solutions: it is

$$x(t) = C_1\,\mathrm{e}^{\lambda_1 t} + C_2\,\mathrm{e}^{\lambda_2 t},$$

where C_1, C_2 are parameters. One can also show that these combinations exhaust the set of possibilities (i.e. there are no solutions of a form other than a linear combination of two exponents).

(2) The auxiliary equation has two complex conjugate roots $\lambda_\pm = \mu \pm i\nu$. This means that

$$x_\pm(t) = \mathrm{e}^{\mu t \pm i\nu t} = \mathrm{e}^{\mu t}\left(\cos\nu t + i\sin\nu t\right),$$

are solutions of the ODE, as are all linear combinations thereof. Forming linear combinations of these, we see that the general solution is given by

$$x(t) = C_1\,\mathrm{e}^{\mu t}\cos\nu t + C_2\,\mathrm{e}^{\mu t}\sin\nu t.$$

Here C_1, C_2 are parameters free to choose and can be fixed by initial conditions.

(3) The third possibility is that auxiliary equation has two coincident real roots, $\lambda_{1,2} = \lambda$, say. In this case we know that

$$x_1(t) = C\,\mathrm{e}^{\lambda t},$$

is a solution, where C is an arbitrary constant. An independent solution is in this case obtained by the method of varying constants. That is one tries to find an independent solution of the form

$$x_2(t) = h(t)x_1(t),$$

in which the constant C above is replaced by an as yet unknown function h. The function h is determined by inserting this ansatz into ODE, which gives

$$\left[a\ddot{h} + (2a\lambda + b)\,\dot{h} + \left(a\lambda^2 + b\lambda + c\right) h\right] \mathrm{e}^{\lambda t} = 0,$$

As the coefficient of h in this equation is $P(\lambda)$ and thus vanishes, and the coefficient of $\dot{h}$ vanishes because $\lambda = -\frac{b}{2a}$ was assumed to be the unique solution of $P(\lambda) = 0$, we are left with the condition

$$\ddot{h} = 0,$$

which gives linear in t solution. Forming linear combinations of x_1 and x_2, we see that the general solution of it is given by

$$x(t) = (C_1 + C_2 t)\,\mathrm{e}^{\lambda t},$$

where as usual C_1 and C_2 are parameters free to choose and can be fixed by initial conditions.

2.4.2. *Inhomogeneous.* We now consider the inhomogeneous ODE with $f(t) \neq 0$. The first thing to note is the following: suppose $x_{\mathrm{ih}}(t)$ is any particular solution of the inhomogeneous equation. Then a solution of the form

$$x(t) = x_{\mathrm{ih}}(t) + x_{\mathrm{h}}(t),$$

with $x_{\mathrm{h}}(t)$ a general solution of the corresponding homogeneous equation is also a solution of the inhomogeneous equation, and this exhausts the possibilities, i.e. there is no solution of the inhomogeneous equation which is not of this form. We already know how to find the $x_{\mathrm{h}}(t)$. So it is sufficient to find a special solution of the inhomogeneous equation. A particular solution of an inhomogeneous equation can be found by the method of varying constants from a solution $x(t) = C_1\,\mathrm{e}^{\lambda t}$ of the homogeneous equation. Thus we attempt a solution $x_{\mathrm{ih}}(t)$ of the inhomogeneous equation of the form

$$x_{\mathrm{ih}}(t) = h(t)\,\mathrm{e}^{\lambda t},$$

with an unknown function F to be determined by inserting the ansatz into ODE. Following the reasoning in case (iii) above, this gives

$$a\ddot{h} + (2a\lambda + b)\,\dot{h} = f(t)\,\mathrm{e}^{-\lambda t}\,.$$

This ODE for h does only involve first and second order derivatives of h and not the function h itself. This can be used to reduce the order of the ODE. Setting $\psi(t) = \dot{h}(t)$, one obtains

$$a\dot{\psi} + (2a\lambda + b)\,\psi = f(t)\,\mathrm{e}^{-\lambda t}\,.$$

This is a first order linear equation and we know how to solve it using integrating factors. Once $\psi(t)$ is obtained along those lines, $h(t)$ follows by a further integration w.r.t. time t, thus finally allowing to write down

$$x_{\mathrm{ih}}(t) = h(t)\,\mathrm{e}^{\lambda t}\,.$$

Occasionally one can be lucky to find a special solution faster by using inspired guesswork as in the following

EXAMPLE Find the solution of the differential equation

$$\ddot{x} + 9x = t,$$

subject to the initial conditions $x(0) = 0$, $\frac{\mathrm{d}\,x}{\mathrm{d}\,t}(0) = 0$. The homogeneous equation corresponding to ODE is

$$\ddot{x}_{\mathrm{h}} + 9x_{\mathrm{h}} = 0.$$

The corresponding auxiliary equation (obtained by substituting the trial solution $\mathrm{e}^{\lambda t}$) is

$$\lambda^2 + 9 = 0,$$

with solution $\lambda = \pm 3i$. It follows that the general solution of homogeneous equation is

$$x_{\mathrm{h}}(t) = C_1 \cos 3t + C_2 \sin 3t,$$

where $C_{1,2}$ are parameters. A particular solution of equation inhomogeneous equation is clearly $x_{\mathrm{ih}}(t) = {}^{t}\!/_{9}$, as follows by inspection. We conclude that the general solution of initial ODE is

$$x(t) = \frac{t}{9} + C_1 \cos 3t + C_2 \sin 3t.$$

where $C_{1,2}$ are parameters. We now pick the solution which satisfies the initial conditions. Imposing the conditions $x(0) = 0$, we obtain $C_1 = 0$, and imposing $\frac{\mathrm{d}\,x}{\mathrm{d}\,t}(0) = 0$ then gives $C_2 = -\frac{1}{27}$. The required solution is therefore

$$x(t) = \frac{3t - \sin 3t}{27}.$$

2.5. Using Fourier Transform to solve ODEs. A very important strategy to solve higher order ODEs is the use of Fourier transform. Let

$$\mathcal{L} = \sum_{k=0}^{n} a_k \frac{\mathrm{d}^k}{\mathrm{d}\,t^k}$$

be a linear differential operator of order n with constant coefficients. We consider a linear ODE of the form

$$\mathcal{L}\left[x\right](t) = \sum_{k=0}^{n} a_k \frac{\mathrm{d}^k\, x(t)}{\mathrm{d}\,t^k} = f(t).$$

Taking Fourier transform of both sides, and using Theorem 2.5 we obtain

$$P\left(\omega\right) \mathcal{F}\left[x\right](\omega) = \mathcal{F}\left[f\right](\omega),$$

where $P(\omega) = \sum_{k=0}^{n} a_k \left(-i\omega\right)^k$ is a polynomial of degree n. The function $x(t)$ now can be found by inverting Fourier transform and is equal to

$$x(t) = \frac{1}{2\pi} \int \frac{\mathcal{F}\left[f\right](\omega)}{P(\omega)} \mathrm{e}^{-i\omega t}\, \mathrm{d}\,\omega.$$

Fourier transform method can be applied to some equations with non-constant coefficients as well.

3. Partial differential equations

Studying the temporal evolution of a system almost always implies the solution of a differential equation in time, as we have seen for ODEs. When the variation is taken also with respect to other variables (i.e. space) then one has to deal

with *partial differential equations* (PDEs). Loosely speaking, a PDE is a relation involving a function u of several real variables $x_1, \dots, x_n$ with its partial derivatives

$$\frac{\partial u}{\partial x_j}, \quad \frac{\partial^2 u}{\partial x_j \partial x_k}, \quad \frac{\partial^3 u}{\partial x_j \partial x_k \partial x_l}, \dots .$$

Every PDE can be written as

$$F\left(\boldsymbol{x}, \frac{\partial u}{\partial x_j}, \frac{\partial^2 u}{\partial x_j \partial x_k}, \dots\right) = 0,$$

where F is some function in multiple variables. General PDE can be rewritten by using multi index formalism.

DEFINITION 3.1. *We call $\alpha = (k_1, k_2, \dots, k_m)$ a multi index of order $|\alpha| = \sum_{j=1}^{m} k_j$. We introduce the notation*

$$\partial_\alpha u = \frac{\partial^k u}{\partial x_1^{k_1} \partial x_2^{k_2} \dots x_m^{k_m}}.$$

Finally, we denote the set of all partial derivatives operators of order k by $\mathcal{D}^k := \{\partial_\alpha \colon |\alpha| = k\}$.

DEFINITION 3.2. *We say that that the PDE is of order k if the highest derivative order of u it contains is k.*

Let us consider now PDEs in the form

$$\mathcal{L}[u]u(\boldsymbol{x}) = f(\boldsymbol{x})$$

where

$$\mathcal{L}[u] = \sum_{j=0}^{k} \sum_{\alpha \colon |\alpha|=j} a_\alpha(\boldsymbol{x}, u, \mathcal{D}^1 u, \dots, \mathcal{D}^j u)\partial_\alpha.$$

DEFINITION 3.3. *We say that a PDE is linear if the operator $\mathcal{L}$ has the form*

$$\mathcal{L} = \sum_{j=0}^{k} \sum_{|\alpha|=j} a_\alpha(\boldsymbol{x})\partial_\alpha.$$

We say that a PDE is semilinear if $\mathcal{L}$ has $a_\alpha \equiv a_\alpha(\boldsymbol{x})$ for $|\alpha| = k$. The PDE is said to be quasilinear if a_α does not depend on derivatives of order $|\alpha|$. Finally, the PDE is homogeneous if $f(\boldsymbol{x}) = 0$, and it is said to be inhomogeneous otherwise.

If the PDE is linear and inhomogeneous and u_{ih} is its solution, then general solution of the PDE can be written as $u = u_{\mathrm{ih}} + u_{\mathrm{h}}$, where u_{h} is a general solution of corresponding homogeneous equation (with $f \equiv 0$).

We list here some important equations appearing in physics and applications. Due to the fact that a natural source for PDEs is dynamics of some physical systems we denote one of the variables as t representing "time".

☞ **Transport equation**: $\partial_t u + c\partial_x u = 0$ is a linear, homogeneous PDE of the first order.

☞ **Burger's equation**: $\partial_t u + u\partial_x u = 0$ is a quasilinear, homogeneous PDE of the first order.

☞ **Eikonal equation**: $\sum_{j=1}^{n} \left|\partial_{x_j} u\right|^2 = \frac{1}{f(\boldsymbol{x})}$ is a non-linear, inhomogeneous PDE of the first order.

☞ **Hamilton-Jacobi equation**: $\partial_t u + H(\boldsymbol{x}, u, \nabla u) = 0$ is a first order PDE, that is usually non-linear, inhomogeneous PDE depending on the Hamiltonian H.

☞ **Korteweg–de Vries equation**: $\partial_t u + (\partial_x u)^3 - 6u\partial_x u = 0$ is a non-linear, homogeneous PDE of the first order.

☞ **Laplace equation**: $\Delta u = 0$ is a linear, homogeneous PDE of the second order.

☞ **Helmholtz equation**: $\Delta u = -\lambda u$ is a linear, homogeneous PDE of the second order.

☞ **Wave equation**: $\partial_t^2 u - c^2 \Delta u = 0$ is a linear, homogeneous PDE of the second order.

☞ **Heat equation**: $\partial_t u - c^2 \Delta u = 0$ is a linear, homogeneous PDE of the second order.

☞ **Schrödinger equation**: $i\partial_t u - \Delta u = 0$ is a linear, homogeneous PDE of the second order.

☞ **Fokker–Planck equation**: $\partial_t u = -\frac{\partial}{\partial x}\left[\mu(t,x)\, u\right] + \frac{\partial^2}{\partial x^2}\left[D(t,x)\, u\right]$, is a linear, homogeneous PDE of the second order.

In general case a PDE is not uniquely solvable and fort his purpose has to be equipped with some boundary conditions on some domain Ω. There are three standard types of boundary conditions one can specify:

Dirichlet boundary conditions: The value of a function u is specified on the boundary of Ω.

Neumann boundary conditions: The value of normal derivative for function u is specified on the boundary of Ω.

Cauchy boundary conditions: A mix of Dirichlet and Neumann boundary conditions are specified for function u on the boundary of Ω.

If the boundary conditions are specified we say that we solve a *boundary value problem for the PDE*. If one of the variables represents time t, then one can give as boundary condition the initial condition, and in this case we solve an *initial value problem*.

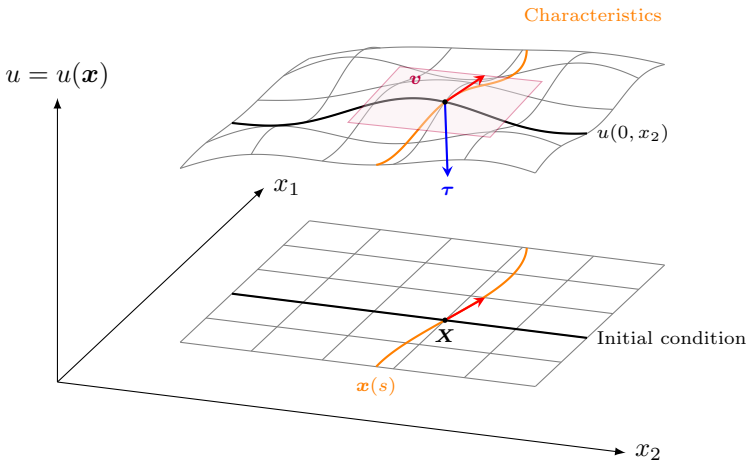
4. Methods of solving PDEs

4.1. Method of characteristics. The method of characteristics is a method for solving linear, semilinear or quasilinear PDEs of the first order, i.e., equations

in the form

$$\sum_{j=1}^{d} a_j\left(\boldsymbol{x}, u\right) \frac{\partial u}{\partial x_j} = f\left(\boldsymbol{x}, u\right), \tag{19}$$

where a_j and f are some known functions of $d+1$ variables. The main goal of the method is to find special curves, called *characteristics*, along which the PDE becomes a family of ODE. Once the ODEs are found and solved along the characteristics curves they can be related to the solution of original PDE. The rational of this idea comes from the observation that we can imagine the solution $s(\boldsymbol{x}, u) \coloneqq u(\boldsymbol{x}) - u = 0$ to be a hypersurface $\mathcal{S} \subset \mathbb{R}^{d+1}$.



Given a point $(\boldsymbol{x}, u(\boldsymbol{x}))$ of this surface, the vector

$$\boldsymbol{\tau} \coloneqq \left(\frac{\partial u}{\partial x_1}, \frac{\partial u}{\partial x_2}, \ldots, \frac{\partial u}{\partial x_d}, -1\right) \equiv (\nabla u, -1)$$

is orthogonal to $\mathcal{S}$ in $\boldsymbol{x}$. On the other hand, Eq. (19) says that the vector $\boldsymbol{v} = (a_1(\boldsymbol{x}, u), \ldots, a_d(\boldsymbol{x}, u), f(\boldsymbol{x}, u))$ is orthogonal to the vector $\boldsymbol{\tau}$: indeed, the equation can be written as $\langle \boldsymbol{v}, \boldsymbol{\tau} \rangle = 0$. This means that $\boldsymbol{v}$ is tangent to $\mathcal{S}$, and the surface $\mathcal{S}$ can be thought as union of many curves going through the surface so that for each $\boldsymbol{x}$ there is only one curve $(\boldsymbol{x}(s), u(s))$ passing through it and solving the set of equations

$$\frac{\mathrm{d}\, x_i}{\mathrm{d}\, s} = a_i(\boldsymbol{x}, u), \text{ for } i = 1, \ldots, d \qquad \frac{\mathrm{d}\, u}{\mathrm{d}\, s} = f(\boldsymbol{x}, u)$$

that can be rewritten in the form of *Lagrange-Charpit equations*

$$\frac{\mathrm{d}\, x_1}{a_1\left(\boldsymbol{x}, u\right)} = \cdots = \frac{\mathrm{d}\, x_d}{a_d\left(\boldsymbol{x}, u\right)} = \frac{\mathrm{d}\, u}{f\left(\boldsymbol{x}, u\right)}. \tag{20}$$

Equations (20) are called *characteristic equations* and describe d-parametric family (coming from d integrations) of characteristic curves. If the PDE is equipped with some initial or boundary data, then one can eliminate all the constants and find unique solution for (19). Otherwise, general solution can be written by assuming that all except one free parameters are expressed as some unknown functions of a last one.

EXAMPLE Consider the initial value problem for **Burgers' equation**

$$\begin{cases} \partial_t u + u\partial_x u = 0, \\ u(x,0) = \phi(x). \end{cases}$$

The characteristic equations are given by

$$\frac{\mathrm{d}\,t}{\mathrm{d}\,s} = 1 \qquad \frac{\mathrm{d}\,x}{\mathrm{d}\,s} = u \qquad \frac{\mathrm{d}\,u}{\mathrm{d}\,s} = 0,$$

with initial conditions

$$t(0) = 0, \qquad x(0) = X, \qquad u(0) = \phi(X), \tag{21}$$

i.e., for $s = 0$ (at the origin of the characteristic curve) x takes the value X, $t = 0$ and $u \equiv \phi(x) = \phi(X)$. All equations are immediately solved as

$$t = s, \qquad x = us + X, \qquad u = \phi(X),$$

implying that $X = x - tu$ and therefore u satisfies the implicit equation

$$u(x,t) = \phi\left(x - u(x,t)t\right).$$

EXAMPLE A radioactive sample consists of a number of identical nuclei, each with a decay probability γ per unit time. We regard the number $n(t)$ of undecayed nuclei at time t as a stochastic process with initial condition $n(0) = n_0$. The probability of having n nuclei at time t evolves according to the following *master equation*

$$\partial_t P(n,t) = \gamma(n+1)P(n+1,t) - \gamma n P(n,t).$$

Let

$$F(z,t) = \sum_{n=0}^{\infty} z^n P(n,t),$$

be a generating function for above probabilities. Then it solves initial value problem

$$\begin{cases} \partial_t F + \gamma(z-1)\partial_z F \quad = 0, \\ F(z,0) = z^{n_0}. \end{cases}$$

The characteristic equations take the form

$$\frac{\mathrm{d}\,t}{1} = \frac{\mathrm{d}\,z}{\gamma(z-1)} = \frac{\mathrm{d}\,F}{0}.$$

Solving the first equation gives

$$t = -\frac{\ln(1-z)}{\gamma} + c \Rightarrow (1-z)\,\mathrm{e}^{-\gamma t} = A.$$

The second equation yields

$$F(z,t) = B.$$

It follows that the characteristic curves are given by $\left(t, 1 - A\,\mathrm{e}^{\gamma t}, B\right)_{t\in\mathbb{R}}$. We can see that along these curves F is a constant and therefore we can put

$$F(z,t) = B = \phi(A) = \phi\left((1-z)\,\mathrm{e}^{-\gamma t}\right),$$

which gives us a general solution. Imposing initial conditions one gets

$$F(z,0) = z^{n_0} = \phi(1-z),$$

and finally

$$F(z,t) = \left(1 + (z-1)\,\mathrm{e}^{-\gamma t}\right)^{n_0}.$$

One can expand the former expression in powers of z to obtain

$$P(n,t) = \binom{n_0}{n} \left(1 - \mathrm{e}^{-\gamma t}\right)^{n_0 - n} \mathrm{e}^{-n\gamma t}.$$

4.2. Fourier transform method. Similarly to the case of ODEs, the main idea of the method is to take Fourier transform of the equation, solve equation in Fourier space and then use the inverse Fourier transform to go back to the original space. However, in the case of PDE one has usually to perform a *partial* Fourier transform, i.e., a Fourier transform with respect to some of the variables, and not all of them. We demonstrate this by solving initial value problem for the heat equation.

EXAMPLE The equation describing d-dimensional **diffusion of heat** is

$$\frac{\partial u(\boldsymbol{x},t)}{\partial t} = \alpha \Delta_{\boldsymbol{x}} u(\boldsymbol{x},t).$$

The solution $u(\boldsymbol{x},t)$ is the temperature in space as a function of time. One could think of a metal bar insulated from outside in such a way that, as a result of the heat flow, its temperature varies with time t and as a function of the position $\boldsymbol{x}$ inside the bar. Here α is a positive constant, called the *thermal diffusivity*. We want to find the solution for $\alpha > 0$ and initial temperature profile $u(\boldsymbol{x},0) = \phi(\boldsymbol{x})$ by Fourier Transform method.

Let us Fourier transform both sides of the equation with respect to space variable $\boldsymbol{x}$ only by introducing the conjugate variable $\boldsymbol{\xi}$

$$\hat{u}(\boldsymbol{\xi},t) = \int_{\mathbb{R}^d} u(\boldsymbol{x},t)\, \mathrm{e}^{i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle}\, \mathrm{d}\,\boldsymbol{x}.$$

As a result, the PDE in $u(\boldsymbol{x},t)$ is mapped into an ODE for $\hat{u}(\boldsymbol{\xi},t)$:

$$\begin{cases} \partial_t \hat{u}(\boldsymbol{\xi},t) = -\alpha \|\boldsymbol{\xi}\|^2 \hat{u}(\boldsymbol{\xi},t), \\ \hat{u}(\boldsymbol{\xi},0) = \hat{\phi}(\boldsymbol{\xi}). \end{cases}$$

For every fixed $\boldsymbol{\xi}$ this is an ODE in variable t with separated variables. Its solution is given by

$$\hat{u}(\boldsymbol{\xi},t) = C(\boldsymbol{\xi})\, \mathrm{e}^{-\alpha t |\boldsymbol{\xi}|^2},$$

where $C(\boldsymbol{\xi})$ can depend on $\boldsymbol{\xi}$ but not t. This constant is fixed by initial condition, and solution in Fourier space takes the form

$$\hat{u}(\boldsymbol{\xi},t) = \hat{\phi}(\boldsymbol{\xi})\, \mathrm{e}^{-\alpha t |\boldsymbol{\xi}|^2}.$$

To find $u(\boldsymbol{x},t)$ we have to invert Fourier transform by using Theorem 2.8. This leads to

$$u(\boldsymbol{x},t) = \frac{1}{(2\pi)^d} \int_{\mathbb{R}^d} \hat{u}(\boldsymbol{\xi},t)\, \mathrm{e}^{-i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle}\, \mathrm{d}\,\boldsymbol{\xi}.$$

Observe that the Fourier transform $\hat{u}(\boldsymbol{\xi},t)$ can be considered as a product of two Fourier transforms, the one of ϕ and a Gaussian $\mathrm{e}^{-\alpha t |\boldsymbol{\xi}|^2}$. If we introduce

$$v(\boldsymbol{x},t) = \frac{1}{(2\pi)^n} \int_{\mathbb{R}^d} \mathrm{e}^{-\alpha t \|\boldsymbol{\xi}\|^2}\, \mathrm{e}^{-i\langle \boldsymbol{\xi}, \boldsymbol{x}\rangle}\, \mathrm{d}\,\boldsymbol{\xi} = \frac{1}{(4\pi\alpha t)^{-\frac{d}{2}}}\, \mathrm{e}^{-\frac{\|\boldsymbol{x}\|^2}{4\alpha t}}.$$

This is called *Green's function for the heat equation*, and solves the equation. The solution for general initial value problem for the heat equation is given in terms of convolution

$$u(\boldsymbol{x},t) = v(\boldsymbol{x},t) * \phi(\boldsymbol{x}) = \int_{\mathbb{R}^d} v(\boldsymbol{x}-\boldsymbol{y},t)\,\phi(\boldsymbol{y})\,\mathrm{d}\,t.$$

For initial condition $\phi(\boldsymbol{x}) = \delta(\boldsymbol{x})$ this lead to a Gaussian answer

$$u(\boldsymbol{x},t) = v(\boldsymbol{x},t) = \frac{1}{(4\pi\alpha t)^{\frac{d}{2}}}\,\mathrm{e}^{-\frac{\|\boldsymbol{x}\|^2}{4\alpha t}}\,.$$

This is the typical form of the solution of a diffusion process: a Gaussian whose variance increases linearly with t and this dependence is mediated by the thermal diffusivity. Thus the width of $u(\boldsymbol{x},t)$ around its mean value ($\boldsymbol{x} = \mathbf{0}$, which is the only value for which $u(\boldsymbol{x},0) \neq 0$) becomes larger with time, meaning that for large enough time also the points x very distant from the origin assume a temperature different from zero.

4.3. Method of variables separation. The method of variables separation is based on two observations:

(1) any linear combination of solutions for linear PDE is a solution as well;
(2) under the assumption that function u factorizes into product of functions depending on single variable some equations can be simplified.

EXAMPLE We consider a boundary value problem for the **Laplace equation** on the unit square $\Omega = [0,1]\times[0,1]$ as an example of method's application. More precisely

$$\begin{cases} \Delta u(x,y) = 0, & (x,y)\in\Omega, \\ u(0,y) = u(1,y) = 0, & y\in[0,1], \\ u(x,0) = x, u(x,1) = 0, & x\in[0,1]. \end{cases}$$

Let us start trying to solve

$$\begin{cases} \Delta u(x,y) = 0 & (x,y)\in\Omega, \\ u(0,y) = u(1,y) = 0 & y\in[0,1] \end{cases}$$

searching for solutions in the form $u(x,y) = \phi(x)\psi(y)$, where ϕ and ψ are some functions of single variable. Laplace equation gives

$$\partial_x^2\phi(x)\psi(y) + \phi(x)\partial_y^2\psi(y) = 0 \Rightarrow \frac{\partial_x^2\phi(x)}{\phi(x)} = -\frac{\partial_y^2\psi(y)}{\psi(y)}.$$

The l.h.s. of the previous equation is a function of x only, but the r.h.s. is a function of y only. Therefore, they can be only equal to constant λ,

$$\partial_x^2\phi(x) = \lambda\phi(x), \quad \partial_y^2\psi(y) = -\lambda\psi(y).$$

A general solution for $\lambda \neq 0$ of the above equations are given by

$$\phi_\lambda(x) = A_1\,\mathrm{e}^{\sqrt{\lambda}x} + A_2\,\mathrm{e}^{-\sqrt{\lambda}x}, \qquad \psi_\lambda(y) = B_1\,\mathrm{e}^{i\sqrt{\lambda}y} + B_2\,\mathrm{e}^{-i\sqrt{\lambda}y}\,.$$

If $\lambda > 0$, then X is given in terms of hyperbolic functions, while Y in terms of trigonometric ones. For $\lambda < 0$ it is vice versa. For $\lambda = 0$ both functions are just linear. What we've got at this point is a 4 parameter family of solutions

$$u_\lambda(x,y) = \begin{cases} \cos\left(\sqrt{\lambda}y+\alpha\right)\left(A\cosh\left(\sqrt{\lambda}x\right) + B\sinh\left(\sqrt{\lambda}x\right)\right), & \lambda > 0, \\ \cos\left(\sqrt{-\lambda}x+\alpha\right)\left(A\cosh\left(\sqrt{-\lambda}y\right) + B\sinh\left(\sqrt{-\lambda}y\right)\right), & \lambda < 0, \\ (x+\alpha)(Ay+B), & \lambda = 0 \end{cases}$$

Boundary conditions yield $\phi_\lambda(0) = \phi_\lambda(1) = 0$ and one can see that they can be satisfied by ϕ_λ only with $\lambda < 0$. Let us take $\lambda = -\omega^2$ for $\omega \in \mathbb{R}_+$, then

$$\cos\alpha = 0 \text{ and } \cos(\alpha+\omega) = 0 \Rightarrow \alpha = \frac{\pi}{2} \text{ and } \omega = \pi k, k \in \mathbb{N}.$$

The corresponding solution is now given by

$$u_k(x,y) = \sin(\pi k x)\left(A_n \cosh(\pi k y) + B_n \sinh(\pi k y)\right).$$

On the second stage of the method we try to find linear combination of functions $u_n(x,t)$ such that it will satisfy boundary conditions in y (boundary conditions in x are satisfied automatically as every u_n satisfies). Let

$$u(x,y) = \sum_{k=1}^{\infty} \sin(\pi k x)\left(A_n \cos(\pi k y) + iB_n \sin(\pi k y)\right).$$

Boundary conditions will yield

$$\sum_{k=1}^{\infty} A_k \sin(\pi n x) = x, \quad \sum_{k=1}^{\infty} \left(A_k \cosh(\pi k) + B_k \sinh(\pi k)\right)\sin(\pi n x) = 0.$$

Both conditions are written as Fourier series expansions and corresponding formulas for coefficients can be used:

$$A_n = 2\int_0^1 \sin(\pi n x)\, x \,\mathrm{d}\, x = \frac{2(-1)^{n+1}}{\pi n}, \quad B_n = \frac{2(-1)^n}{\pi n}\coth(\pi n).$$

Combining all the above we obtain solution for the initial problem in the form

$$u(x,y) = \sum_{n=1}^{\infty} \frac{2(-1)^n}{\pi n}\sin(\pi n x)\left(\coth(\pi n)\sinh(\pi n y) - \cosh(\pi n y)\right).$$

EXAMPLE We exemplify here all methods above calculating the time-dependent solution of the **Fokker-Planck equation for the Ornstein-Uhlenbeck process**, modelling the velocity of a Brownian particle of mass m, immersed in a fluid at absolute temperature T, and with damping coefficient γ,

$$\frac{\partial}{\partial t}P(v,t) = \gamma\frac{\partial}{\partial v}\left[vP(v,t)\right] + \frac{\gamma T}{m}\frac{\partial^2}{\partial v^2}P(v,t),$$

with initial condition $P(v,t_0) = \delta(v - v_0)$. We can first consider the Fourier transform in variable v given by

$$\hat{P}(u,t) = \int P(v,t)\,\mathrm{e}^{ivu}\,\mathrm{d}\, v.$$

After multiplication of FP equation by e^{ivu} and integrating with respect to v we obtain

$$\frac{\partial}{\partial t}\hat{P}(u,t) = -\gamma u\frac{\partial}{\partial u}\hat{P}(u,t) - \gamma u^2\frac{\gamma T}{m}\hat{P}(u,t).$$

The last equation is a linear, inhomogeneous PDE and we solve it by using the method of characteristics:

$$\frac{\mathrm{d}\, t}{1} = \frac{\mathrm{d}\, u}{\gamma u} = -\frac{m\,\mathrm{d}\,\hat{P}}{\gamma^2 u^2 T\hat{P}}.$$

The first equation is easily solved as

$$u = C_1\,\mathrm{e}^{\gamma t}.$$

The second equation is solved by

$$\hat{P}(u,t) = C_2 \, \mathrm{e}^{-\frac{\gamma k T}{2m} u^2} .$$

It follows that the general solution of the PDE can be written as

$$\hat{P}(u,t) = \phi\left(u \, \mathrm{e}^{-\gamma t}\right) \mathrm{e}^{-\frac{\gamma T}{2m} u^2},$$

for an unknown function ϕ. Such a function can be fixed by the initial conditions. Indeed, the initial value can be easily calculated and is given by

$$\hat{P}\left(u, t_0\right) = \int \delta\left(v - v_0\right) \mathrm{e}^{iuv} \, \mathrm{d}\, v = \mathrm{e}^{iuv_0} .$$

so that

$$\phi\left(u \, \mathrm{e}^{-\gamma t_0}\right) \mathrm{e}^{-\frac{\gamma T}{2m} u^2} = \mathrm{e}^{iuv_0} \Rightarrow \phi(u) = \exp\left(iu \, \mathrm{e}^{\gamma t_0} \, v_0 + \frac{\gamma T \, \mathrm{e}^{2\gamma t_0}}{2m} u^2\right).$$

Combining the above we obtain

$$\hat{P}(u,t) = \exp\left(iu \, \mathrm{e}^{-\gamma(t-t_0)} \, v_0 - \frac{\gamma k T \left(1 - \mathrm{e}^{-2\gamma(t-t_0)}\right)}{2m} u^2\right).$$

Taking inverse Fourier transform we can calculate function $P\left(v,t\right)$

$$\begin{aligned} P\left(v,t\right) &= \frac{1}{2\pi} \int \hat{P}(u,t) \, \mathrm{e}^{-iuv} \, \mathrm{d}\, u \\ &= \sqrt{\frac{m}{2\pi\gamma T \left(1 - \mathrm{e}^{-2\gamma(t-t_0)}\right)}} \exp\left\{ \frac{-m\left(v - v_0 \, \mathrm{e}^{-\gamma(t-t_0)}\right)^2}{2T\left(1 - \mathrm{e}^{-2\gamma(t-t_0)}\right)} \right\}. \end{aligned}$$

Exercises

(1) Find the solutions to the following first order ODEs
   (a) $\dot{x}(t) = 6t^2 x(t)$.
   (b) $t\left(t+1\right)\dot{x}(t) - \left(t+2\right)x(t) = t^3\left(2t-3\right)$.
   (c) $\frac{\mathrm{d}\, y(x)}{\mathrm{d}\, x} = \frac{\sin x}{y(x)\cos y(x)}$.
   (d) $x\frac{\mathrm{d}\, y(x)}{\mathrm{d}\, x} + y(x) = x^2 + 1$.
   (e) $\frac{\mathrm{d}\, y(x)}{\mathrm{d}\, x} + \tan(x) y(x) = \cos^2(x)$ with condition $y(0) = 2$.

(2) Find the solutions to the following second-order ODEs
   (a) $\ddot{x}(t) + 11\dot{x}(t) + 24x(t) = 0$.
   (b) $\frac{\mathrm{d}^2 y(x)}{\mathrm{d}\, x^2} + 4\frac{\mathrm{d}\, y(x)}{\mathrm{d}\, x} + 4y = 0$.
   (c) $\frac{\mathrm{d}^2 y(x)}{\mathrm{d}\, x^2} - 8\frac{\mathrm{d}\, y(x)}{\mathrm{d}\, x} + 17y = 0, \quad y(0) = -4, y'(0) = -1$.
   (d) $\ddot{x}(t) + 9x(t) = t, \quad x(0) = 0, \dot{x}(0) = 0$.
   (e) $\frac{\mathrm{d}^2 y(x)}{\mathrm{d}\, x^2} + 3\frac{\mathrm{d}\, y(x)}{\mathrm{d}\, x} + 2y = \mathrm{e}^{-x}, \quad y(0) = -4, y'(0) = -1$.

(3) The time evolution of the magnetisation m of a ferromagnetic material in the vicinity of the critical temperature T_c is described by the dynamical system

$$\frac{\mathrm{d}\, m(t)}{\mathrm{d}\, t} = f\left(m(t)\right) = am(t) - m^3(t),$$

where $a = \frac{T_c - T}{T_c}$ and T is the temperature.

(a) Sketch the phase portrait for the cases $T > T_c$ and $T < T_c$. Write down the fixed points of the motion and the invariant open sets of the dynamics for both $T > T_c$ and $T < T_c$; discuss the stability of the fixed points in both cases.
(b) Show, for $T < T_c$ - without using the exact solution of the differential equation - that, if $m(0) = \sqrt{a}/2$, the system will not reach $x = \sqrt{a}$ in finite time.
(c) Show, for $T < T_c$ the exact solution of this equation, with initial condition $m(0) = \sqrt{a}/2$ is

$$m(t) = \sqrt{\frac{a}{1 + 3\,\mathrm{e}^{-2at}}}.$$

(d) For $T > T_c$ and for $T = T_c$ give solutions of the asymptotic equation of motion in vicinity of $m = 0$, assuming $m(0) = m_0 > 0$, but small.

(4) A second order dynamical system is described by the differential equations

$$\begin{cases} \dot{x}(t) &= y(t) + x(t) f\left(r(t)\right), \\ \dot{y}(t) &= x(t) + y(t) f\left(r(t)\right). \end{cases}$$

where $r(t) = \sqrt{x^2(t) + y^2(t)}$. Show that the system is separable in hyperbolic coordinates (r, θ) where $x = r\cosh\theta, y = r\sinh\theta$ and in particular that $\dot{r}(t) = r(t) f\left(r(t)\right)$ and $\dot{\theta}(t) = 1$.

(5) Consider the second order dynamical system described by

$$\begin{cases} \dot{x} &= f_1(x, y) = 2xy, \\ \dot{y} &= f_2(x, y) = 1 - x^2 - y^2. \end{cases}$$

Find the null-clines of f_1 and f_2. Use them to find the fixed points of the system. Sketch the phase portrait including the null-clines, using the usual arrow representation of the phase- flow. Discuss the nature and stability of the fixed points.

(6) Given the second order dynamical system

$$\begin{cases} \dot{x} &= f_1(x, y) = \mathrm{e}^{-x-y} - 1, \\ \dot{y} &= f_2(x, y) = \sin(x - y). \end{cases}$$

(a) Determine the null-clines of f_1 and f_2 and the fixed points of the system.
(b) Compute the Jacobian $\boldsymbol{J_f}$ associated with the dynamical system and evaluate it at the fixed points.
(c) Determine the eigenvalues of the Jacobian and thereby the Jordan canonical form $\boldsymbol{J}^*$ corresponding to $\boldsymbol{J_f}$.

(7) Using method of variables separation solve forced heat equation on a one dimensional strip

$$\partial_t u - a^2 \partial_x^2 u = \mathrm{e}^{-t}, \quad x \in [0, 1], \quad t > 0$$

with boundary conditions

$$\begin{cases} u(0, t) = 0, \\ u(1, t) = 1. \end{cases}$$

and initial condition

$$u(x,0) = x(1-x).$$

(8) Using Fourier transform method solve wave equation in d dimensions

$$\partial_t^2 u = c^2 \Delta_{\boldsymbol{x}} u, \quad \boldsymbol{x} \in \mathbb{R}^d,\ t > 0.$$

with initial conditions

$$u(\boldsymbol{x},t) = \phi(\boldsymbol{x}).$$

Find the corresponding Green's function for the wave equation.

(9) Using Fourier transform method solve Laplace equation in half plane

$$\Delta u(x,y) = 0, \quad y > 0, \quad x \in \mathbb{R},$$

with Cauchy boundary conditions

$$u_y - \alpha u|_{y=0} = \phi(x).$$