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Department of Physics and Astronomy G. Galilei
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course notes
OF
MODELS OF THEORETICAL PHYSICS

Professor Sandro Azaele, Academic Year 2024/2025.

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A note to the reader

This document comprehensively covers the material presented in the course Models of Theoretical Physics, held during the first semester of the 2024/25 academic year. It is intended for students enrolled in the master's programs in both Physics of Matter and Physics of Data. The document is the result of a collaborative effort among several students and is freely distributed to all students in the course, both this year and in the future. We hope it serves as a valuable study aid. Please note, however, that these notes were prepared by students and have not been reviewed by the course instructor. If you notice any conceptual errors or typographical mistakes, please reach out to one of the contributors at the addresses listed below. We will gladly address any corrections. Wishing you a productive and enjoyable learning journey!

The students:

Pietro Marcazzan, pietro.marcazzan.1@studenti.unipd.it
Leonardo Pieripolli, leonardo.pieripolli@studenti.unipd.it
Matteo Vezzoli, matteo.vezzoli@studenti.unipd.it
Miriam Zara, miriam.zara@studenti.unipd.it

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Chapter 1

Mathematical tools

1.1 Gaussian integrals

Let's consider the following gaussian distribution (PDF[1]):

> **Definition 1: Gaussian Distribution PDF**
>
> $$p(x) = c \cdot e^{-\frac{ax^2}{2}}, \quad a > 0$$

where $p(x)$ must be normalized in $(-\infty, +\infty)$. Knowing that the simplest gaussian integral gives the following:

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}} \, \mathrm{d}x = \sqrt{\frac{2\pi}{a}}, \forall a > 0 \tag{1.1}$$

We can affirm that

$$\int_{-\infty}^{+\infty} p(x) \, \mathrm{d}x \overset{!}{=} 1 \implies c \int_{-\infty}^{\infty} e^{-a\frac{x^2}{2}} \, \mathrm{d}x = c \cdot \sqrt{\frac{2\pi}{a}} = 1 \implies c = \sqrt{\frac{a}{2\pi}}$$

Let's now consider a more general gaussian integral :

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2} + bx} \, \mathrm{d}x = ? \tag{1.2}$$

Which we can solve by shifting the minimum of the exponent through an appropriate *change of of variables*:

$$\frac{\mathrm{d}}{\mathrm{d}x}\left(-\frac{ax^2}{2} + bx\right) = -ax + b \overset{!}{=} 0 \implies x = \frac{b}{a}, \quad b \in \mathbb{R} \text{ for now}$$

We thus found the minimum at $\frac{b}{a}$ and can now define $y = x - \frac{b}{a}$, such as to obtain a new exponent with minimum at $y = 0$:

$$-\frac{ax^2}{2} + bx = \frac{-ay^2}{2} + \frac{b}{2a} \quad, \quad \mathrm{d}y = \mathrm{d}x$$

Inserting it in expression 1.2 gives:

$$\int_{-\infty}^{+\infty} e^{-\frac{ay^2}{2} + \frac{b^2}{2a}} \, \mathrm{d}y = e^{\frac{b^2}{2a}} \cdot \int_{-\infty}^{+\infty} e^{-\frac{ay^2}{2}} \, \mathrm{d}y$$

$$\overset{1.1}{=} \sqrt{\frac{2\pi}{a}} e^{\frac{b^2}{2a}}$$

---

[1]Probability Density Function

which leads to a more general gaussian integral:

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}+bx}\,\mathrm{d}x = \sqrt{\frac{2\pi}{a}}\,e^{\frac{b^2}{2a}} \tag{1.3}$$

If we allow $b \in \mathbb{C}$, we can calculate for $b = it$, $t \in \mathbb{R}$:

$$\varphi(t) = \sqrt{\frac{a}{2\pi}} \int_{-\infty}^{+\infty} \mathrm{d}x\, e^{-\frac{ax^2}{2}+ixt} = e^{\frac{-t^2}{2a}}$$

(which is equivalent to taking the Fourier transform of the gaussian PDF).
Such result can also be reached through the following reasoning: taking the derivative with respect to t, we can calculate

$$
\begin{aligned}
\frac{\mathrm{d}\varphi}{\mathrm{d}t} &= \frac{\mathrm{d}}{\mathrm{d}t}\left(\sqrt{\frac{a}{2\pi}}\int_{-\infty}^{+\infty}\mathrm{d}x\, e^{ixt-\frac{a}{2}x^2}\right) \\
&= \sqrt{\frac{a}{2\pi}}\int_{-\infty}^{+\infty}\mathrm{d}x\, ix\, e^{ixt-\frac{a}{2}x^2} \\
&= \frac{-i}{\sqrt{2\pi a}}\int_{-\infty}^{+\infty}\mathrm{d}x\, e^{ixt}\frac{\mathrm{d}}{\mathrm{d}x}\left(e^{\frac{a}{2}x^2}\right) \\
&= \frac{-t}{\sqrt{2\pi a}}\int_{-\infty}^{+\infty}\mathrm{d}x\, e^{ixt-\frac{a}{2}x^2} \\
&= \frac{-t}{a}\varphi(t)
\end{aligned}
$$

Where we used integration by parts to obtain the fourth expression and the second from

$$\frac{\mathrm{d}}{\mathrm{d}t}\int f(x,t)\,\mathrm{d}x = \int \frac{\partial}{\partial t}f(x,t)\,\mathrm{d}x \ ,$$

which holds if f and $\partial f/\partial t$ are continuous and uniformly bounded:

$$
\begin{aligned}
|f(x,t)| < A(x), \qquad\qquad & \int A(x)\,\mathrm{d}x < \infty \\
|\partial_t f(x,t)| < B(x), \qquad\qquad & \int B(x)\,\mathrm{d}x < \infty
\end{aligned}
$$

We thus reached

$$\frac{\mathrm{d}\varphi}{\mathrm{d}t} = -\frac{t}{a}\varphi(t)$$

This differential equation is solved by separation of variables to obtain

$$\varphi(t) = c \cdot e^{-\frac{t^2}{2a}} = c \cdot e^{\frac{b^2}{2a}}$$

with $\varphi(0) = 1 \implies c = 1$, following from previous definitions of φ.

1.2 Characteristic function

> **Definition 2: Characteristic Function**
>
> Given a PDF $p(x)$, its *characteristic function* (CF) is defined as
>
> $$\varphi(k) = \int e^{ikx}\, p(x)\, \mathrm{d}x \equiv \left\langle e^{ikx} \right\rangle \tag{1.4}$$

Where the general definition of expected value was used:

$$\langle f(x) \rangle \equiv \int f(x)\, p(x)\, \mathrm{d}x$$

Note that $\varphi(k)$ has the following property:

$$\frac{\mathrm{d}\varphi}{\mathrm{d}k} = \int (ix)\, e^{ikx}\, p(x)\, \mathrm{d}x \implies -i\, \frac{\mathrm{d}\varphi}{\mathrm{d}k}\bigg|_{k=0} = \int x\, p(x)\, \mathrm{d}x \equiv \langle x \rangle$$

which can be generalized for higher order derivatives:

$$(-i)^n\, \frac{\mathrm{d}^n \varphi}{\mathrm{d}k^n}\bigg|_{k=0} = \int x^n\, p(x)\, \mathrm{d}x \equiv \langle x^n \rangle \quad \forall\, n \in \mathbb{N} \tag{1.5}$$

We now ask ourselves what is the characteristic function of a *gaussian PDF*. Using the solution of equation 1.3 with $b = it$, $t \in \mathbb{R}$ and $a = 1/\sigma^2$, we get

$$\frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} e^{\frac{-x^2}{2\sigma^2} - ikx}\, \mathrm{d}x = e^{-\frac{\sigma^2 k^2}{2}} \tag{1.6}$$

> **Example 1: Higher order CF for a gaussian distribution**
>
> alculating the CF for every order of derivation will prove to be useful so by applying equation 1.5 to the gaussian characteristic function one can show that
>
> $$-i\, \frac{\mathrm{d}}{\mathrm{d}k}\left(e^{-\frac{\sigma^2 k^2}{2}} \right)\bigg|_{k=0} = \langle x \rangle = \frac{1}{\sqrt{2\pi\sigma^2}} \int_{-\infty}^{+\infty} e^{-\frac{x^2}{2\sigma^2}}\, x\, \mathrm{d}x = 0$$
>
> as the product of an odd function and an even function is odd, their integral over a symmetric domain is null. Following the same reasoning, one can affirm that
>
> $$\langle x^n \rangle = (-i)^n\, \frac{\mathrm{d}^n}{\mathrm{d}k^n}\bigg|_{k=0} e^{\frac{-\sigma^2 k^2}{2}} = 0 \quad \forall\, n\, \text{odd}$$
>
> For even n, we can proceed by induction in the following way, starting from equation 1.1, deriving both sides by a and simplifying:
>
> $$\int_{\mathbb{R}} e^{-ax^2}\, \mathrm{d}x \quad = \frac{\sqrt{2\pi}}{a^{1/2}}$$
>
> $$\int_{\mathbb{R}} x^2\, e^{-ax^2}\, \mathrm{d}x = \frac{3\sqrt{2\pi}}{a^{3/2}}$$
>
> $$\int_{\mathbb{R}} x^4\, e^{-ax^2}\, \mathrm{d}x = \frac{5 \cdot 3\sqrt{2\pi}}{a^{5/2}}$$
>
> $$\int_{\mathbb{R}} x^6\, e^{-ax^2}\, \mathrm{d}x = \frac{7 \cdot 5 \cdot 3\sqrt{2\pi}}{a^{7/2}}$$
>
> $$\vdots \qquad\qquad \vdots$$

Doing so clearly shows the inductive process and, by remembering equation 1.5, we can affirm that

$$(-i)^n \left. \frac{\mathrm{d}^n \varphi}{\mathrm{d}k^n} \right|_{k=0} = \int_{\mathbb{R}} x^n e^{-ax^2} \, \mathrm{d}x = \frac{(n-1)!! \sqrt{2\pi}}{a^{(n+1)/2}} \quad \forall \, n \text{ even}$$

where the !! denotes the double factorial, defined as $n!! = n \cdot (n-2) \cdot (n-4) \ldots 2$ or 1

Example 2: Variance implications on gaussian PDFs

$$\langle x^2 \rangle = -\frac{\mathrm{d}2}{\mathrm{d}k^2} \left(e^{-\frac{\sigma^2 k^2}{2}} \right) \Bigg|_{k=0}$$

$$= \sigma^2 \left(1 + \sigma^2 k^2 \right) e^{-\frac{\sigma^2 k^2}{2}} \Bigg|_{k=0}$$

$$= \sigma^2$$

Which is the same result we would've obtained through the usual $\sigma^2 = \langle x^2 \rangle - \langle x \rangle^2$

$$\langle x^4 \rangle = -\frac{\mathrm{d}^4}{\mathrm{d}k^4} e^{-\frac{\sigma^2 k^2}{2}} \Bigg|_{k=0}$$

$$= \sigma^4 \left(3 - 6\sigma^2 k^2 + k^4 \sigma^4 \right) e^{-\frac{\sigma^2 k^2}{2}} \Bigg|_{k=0}$$

$$= 3\sigma^4$$

Exercise 1: CF of a uniform distribution

Given a random variable x drawn from a uniform distribution $U([a,b])$, calculate the CF of $p(x)$ where

$$p(x) = \begin{cases} 1 & \frac{1}{b-a} \in [a,b] \\ 0 & \text{elsewhere} \end{cases}$$

Exercise 2: C.F of a γ-distribution

Given a random variable x drawn from a γ-distribution $\gamma(\alpha, \beta)$, with $\alpha > 0$, $\beta > 0$ prove that such distribution is normalized and calculate the CF of $q(x)$ where

$$q(x) = \gamma(\alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1} e^{-\beta x} \qquad (0 \le x \le \infty \text{ or } x \in \mathbb{R}^+)$$

where $\Gamma(\alpha)$ represent the gamma function defined as usual:

$$\Gamma(z) = \int_0^\infty t^{z-1} e^{-t} \, \mathrm{d}t$$

Exercise 3: CF of a general gaussian distribution

Given a random variable x drawn from a gaussian distribution $\mathcal{N}(\mu, \sigma^2)$, calculate its CF Remember that such distribution is defined as

$$\mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}$$

1.3 Multidimensional gaussian integrals

Given the following expression

$$\int_{-\infty}^{+\infty} \mathrm{d}x_1 \int_{-\infty}^{+\infty} \mathrm{d}x_2 \; e^{\left(-\frac{3}{2}(x_1^2 + x_2^2) + x_1 x_2\right)} = ?$$

How do we approach such integrals? A possible way is to rewrite the exponent in terms of a matrix product: $-\frac{1}{2}\vec{x}^\mathsf{T} \mathbf{A} \vec{x}$ where $\vec{x}^\mathsf{T} \mathbf{A} \vec{x} = \sum_{ij} x_i A_{ij} x_j$.

> **Exercise 4**
>
> Write down the exponent of the example problem in matrix product notation and find $\mathbf{A}$.

The general problem we want to solve is

$$Z(\mathbf{A}) = \int_{\mathbb{R}^n} \mathrm{d}x^n \; e^{-\frac{1}{2}\vec{x}^\mathsf{T} \mathbf{A} \vec{x}} = ? \tag{1.7}$$

$$\vec{x} \equiv (x_1, x_2, \ldots, x_n)$$

We start by observing that $\mathbf{A}$ is diagonalizable with strictly positive eigenvalues. $\mathbf{A}$ is also symmetric $\Rightarrow \exists$ orthogonal matrix $\mathbf{O}$ ($\mathbf{OO}^\mathsf{T} = \mathbf{O}^\mathsf{T}\mathbf{O} = \mathbb{1}$) such that $\vec{y} = \mathbf{O}\vec{x}$ and $\mathbf{OAO}^\mathsf{T} = \mathbf{\Lambda}$ with

$$\mathbf{\Lambda} = \begin{pmatrix} \lambda_1 & 0 & \cdots & 0 \\ 0 & \lambda_2 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & \cdots & \lambda_n \end{pmatrix}$$

Therefore

$$\vec{x}^\mathsf{T} \mathbf{A} \vec{x} = \vec{x}^\mathsf{T} \mathbf{O}^\mathsf{T} \mathbf{\Lambda} \mathbf{O} \vec{x} = \vec{y}^\mathsf{T} \mathbf{\Lambda} \vec{y}$$

and

$$\vec{y}^\mathsf{T} \mathbf{\Lambda} \vec{y} = \sum_{ij} y_i \lambda_i \delta_{ij} y_j = \sum_i \lambda_i y_i^2$$

Inserting this into $Z(\mathbf{A})$:

$$Z(\mathbf{A}) = \int_{\mathbb{R}^n} \mathrm{d}x^n \; e^{-\frac{1}{2}\vec{x}^\mathsf{T} \mathbf{A} \vec{x}}$$

$$= \int_{\mathbb{R}^n} \mathrm{d}y^n \underbrace{\left\| \frac{\partial \vec{x}}{\partial \vec{y}} \right\|}_{=1} e^{-\frac{1}{2}\vec{y}^\mathsf{T} \mathbf{\Lambda} \vec{y}}$$

$$\overset{1.3}{=} \int_{\mathbb{R}^n} \mathrm{d}y^n \; e^{-\frac{1}{2}\sum_i \lambda_i y_i^2}$$

$$= \prod_i^n \int_{\mathbb{R}} \mathrm{d}y_i \; e^{-\frac{1}{2}\lambda_i y_i^2}$$

$$\overset{1.1}{=} \prod_i^n \sqrt{\frac{2\pi}{\lambda_i}}$$

$$= \frac{(2\pi)^{n/2}}{\sqrt{\lambda_1 \ldots \lambda_n}}$$

where

$$\left\|\frac{\partial \vec{x}}{\partial \vec{y}}\right\| = \det(\mathbf{O}^{\mathsf{T}}) = 1$$

is determinant of the Jacobian, which is unitary because the determinant of an orthogonal matrix is always 1 (or -1). Using

$$\begin{aligned}
\det(\mathbf{A}) &= \det(\mathbf{O}^{\mathsf{T}}\boldsymbol{\Lambda}\mathbf{O}) \\
&= \det(\boldsymbol{\Lambda})\det(\mathbf{O})^2 \\
&= \det(\boldsymbol{\Lambda}) = \lambda_1 \dots \lambda_n \ ,
\end{aligned}$$

We finally get

$$Z(\mathbf{A}) = \frac{(2\pi)^{n/2}}{\sqrt{\det(\mathbf{A})}} \tag{1.8}$$

Exercise 5

Show that

$$\iint_{\mathbb{R}^2} \mathrm{d}x_1\,\mathrm{d}x_2\,e^{\left(-\frac{3}{2}(x_1^2+x_2^2)+x_1 x_2\right)} = \frac{\pi}{\sqrt{2}}$$

Exercise 6

Let

$$p(x,y) = \frac{\sqrt{\det(\mathbf{A})}}{2\pi}\,e^{-\frac{1}{2}a_{11}x^2 + 2a_{12}xy + a_{22}y^2}$$

where

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad a_{11},\,a_{22} > 0, \quad a_{12} = a_{21}$$

Show that $p(x,y)$ is normalized and that $\int p(x,y)\,\mathrm{d}y$ is still a gaussian PDF. Find the corresponding variance of the random variable x.

An even more general problem is the following:

$$Z(\mathbf{A},\vec{b}) = \int_{\mathbb{R}^n} \mathrm{d}x^n\,e^{-\frac{1}{2}\vec{x}^{\mathsf{T}}\mathbf{A}\vec{x} + \vec{x}^{\mathsf{T}}\vec{b}} = ? \tag{1.9}$$

Once again we shift the minimum as done to solve equation 1.2. We must first find such minimum:

$$\boldsymbol{\nabla}_x\left(-\frac{1}{2}\vec{x}^{\mathsf{T}}\mathbf{A}\vec{x} + \vec{x}^{\mathsf{T}}\vec{b}\right) = -\mathbf{A}\vec{x} + \vec{b} \overset{!}{=} 0$$

We introduce $\vec{y} = \vec{x} - \mathbf{A}^{-1}\vec{b}$, made possible by the fact that $\det(\mathbf{A}) \neq 0$ due to the previous assumptions on $\mathbf{A}$ itself:

$$-\frac{1}{2}\vec{x}^{\mathsf{T}}\mathbf{A}\vec{x} + \vec{x}^{\mathsf{T}}\vec{b} = \dots = -\frac{1}{2}\vec{y}^{\mathsf{T}}\mathbf{A}\vec{y} + \frac{\vec{b}^{\mathsf{T}}\mathbf{A}^{-1}\vec{b}}{2}$$

Hence

$$Z(\mathbf{A},\vec{b}) = \int_{\mathbb{R}^n} \mathrm{d}\vec{y}\,e^{-\frac{1}{2}\vec{y}^{\mathsf{T}}\mathbf{A}\vec{y} + \frac{1}{2}\vec{b}^{\mathsf{T}}\mathbf{A}^{-1}\vec{b}} \overset{1.7}{=} (\mathbf{A},\vec{0})e^{\frac{1}{2}\vec{b}^{\mathsf{T}}\mathbf{A}^{-1}\vec{b}}$$

and using equation 1.8 we get:

$$Z(\mathbf{A}, \vec{b}) = \frac{(2\pi)^{n/2}}{\sqrt{\det(\mathbf{A})}} \, e^{\frac{1}{2}\vec{b}^{\mathsf{T}}\mathbf{A}^{-1}\vec{b}} \tag{1.10}$$

Another way in which this relations is usually referred to is the following, also known as the **Hubbard-Stratonovich transformation**

> **Definition 3: Hubbard-Stratonovich transformation**
>
> $$e^{\frac{1}{2}\vec{b}^{\mathsf{T}}\mathbf{A}^{-1}\vec{b}} = \frac{\sqrt{\det(A)}}{(2\pi)^{n/2}} \int_{\mathbb{R}} \mathrm{d}^n x \, e^{-\frac{1}{2}\vec{x}^{\mathsf{T}}\mathbf{A}\vec{x} + \vec{x}^{\mathsf{T}}\vec{b}}$$

Equation 1.10 also allows us to find the *characteristic function* of a *multivariate gaussian PDF*:

$$p(\vec{x}) = \frac{1}{Z(\mathbf{A}, \vec{0})} e^{-\frac{1}{2}\vec{x}^{\mathsf{T}}\mathbf{A}^{-1}\vec{x}}$$

With $\vec{b} \to i\vec{k}$ and the mentioned equation 1.10:

$$\varphi(\vec{k}) = \int_{\mathbb{R}^n} \mathrm{d}^n x \, p(\vec{x}) e^{i\vec{k}\cdot\vec{x}}$$

$$= e^{-\frac{\vec{k}^{\mathsf{T}}\mathbf{A}^{-1}\vec{k}}{2}} \tag{1.11}$$

1.3.1 The meaning of $\mathbf{A}^{-1}$

We now calculate the s-point correlation function with the help of the characteristic function from equation 1.5

$$\underbrace{\langle x_i \, x_j \ldots x_l \rangle}_{s \text{ variables}} = \int_{\mathbb{R}^s} \mathrm{d}^s x \; x_i \, x_j \ldots x_l \, p(\vec{x}) \overset{1.5}{=} (-i)^s \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} \cdots \frac{\partial}{\partial k_l} \varphi(\vec{k}) \Big|_{\vec{k}=0}$$

The former equation is general. If we try to calculate the specific case for the 2-point correlation function we can reach the following

$$\langle x_i \, x_j \rangle = (-i)^2 \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} \varphi(\vec{k}) \Big|_{\vec{k}=0}$$

$$= (-i)^2 \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} e^{-\frac{1}{2}\vec{k}^{\mathsf{T}}\mathbf{A}^{-1}\vec{k}} \Big|_{\vec{k}=0}$$

$$= \ldots$$

$$= \left(\mathbf{A}^{-1}\right)_{ij} \tag{1.12}$$

$\mathbf{A}^{-1}$ is thus the 2-point correlation function between a pair of gaussian random variables.

> **Exercise 7**
>
> Do the calculations that leads to equation 1.12.

When $\mathbf{A}^{-1}$ is a diagonal matrix, the variables are said to be *uncorrelated*. In the previous example:

$$\mathbf{A}^{-1} = \frac{1}{8} \begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix}$$

Hence

$$\left\langle x_1^2 \right\rangle = \frac{3}{8} = \left\langle x_2^2 \right\rangle, \quad \left\langle x_1\, x_2 \right\rangle = \frac{1}{8} = \left\langle x_2\, x_1 \right\rangle$$

Note: Because of symmetry, the s-point correlation for any odd integer s is 0 (gaussian remains unchanged if $\vec{x} \to -\vec{x}$).

When we want to calculate $\langle x_i\, x_j \ldots x_l \rangle$, should we always calculate all the derivatives as in equation 1.3.1? If the variables are gaussian, there's a shortcut, given by the following theorem:

Definition 4: Wicks's Theorem

Any correlation between an even number of gaussian random variables can be written as a sum of products of 2-point correlation functions ($\mathbf{A}^{-1}$):

$$\underbrace{\left\langle x_i\, x_j \ldots x_y\, x_z \right\rangle}_{s \text{ variables}} = \sum_P \left(\mathbf{A}^{-1} \right)_{i_p\, j_p} \ldots \left(\mathbf{A}^{-1} \right)_{y_p\, z_p} \tag{1.13}$$

Where the sum runs over all pairings of s indices, i.e. over all ways of grouping s even indices i, j, $\ldots$, y, z into pairs (counting the pairs even when indexes are equal). For s variables there are $(s-1)!!$ possible pairings.

For instance:

$$\langle x_a x_b x_c x_d \rangle = \underbrace{\langle x_a\, x_b \rangle}_{(\mathbf{A}^{-1})_{ab}} \underbrace{\langle x_c\, x_d \rangle}_{(\mathbf{A}^{-1})_{cd}} + \langle x_a\, x_c \rangle \langle x_b\, x_d \rangle + \langle x_a\, x_d \rangle \langle x_b\, x_c \rangle$$

Exercise 8

From the previous case, show with the help of *Wick's theorem* that

$$\left\langle x_1^2\, x_2^2 \right\rangle = \frac{3}{8} \cdot \frac{3}{8} + \frac{1}{8} \cdot \frac{1}{8} + \frac{1}{8} \cdot \frac{1}{8} = \frac{11}{64}\ ,$$

$$\left\langle x_1^4 \right\rangle = 3 \left(\frac{3}{8} \right)^2 = \left\langle x_2^4 \right\rangle, \quad \left\langle x_1\, x_2^2 \right\rangle = 0$$

1.4   Properties of the characteristic function

The characteristic function of a probability density function is a powerful tool that allows easier results for otherwise tedious properties or calculations of the PDF.

1.4.1   Sum of random variables

From the most general case, given two *random variables*[2] x_1, x_2, their joint probability distribution can be written as $p(x_1, x_2)$, meaning the probability of getting values x_1 and x_2 for the same draw; if the two random variables are independent, probability can be separated as $p(x_1, x_2) = q_1(x_1) q_2(x_2)$, where q_1, q_2 are the single variable probability density functions for x_1 and x_2 respectively; furthermore, if the two variables are also identically distributed, the probabilities are the same $q_1 = q_2 = q$ so $p(x_1, x_2) = q(x_1) q(x_2)$. This can be easily extended to the n dimensional case

$$p(x_1, x_2, ..., x_n) = \underbrace{\prod_{i=1}^{n} q_i(x_i)}_{\text{if independents r.v.s}} = \overbrace{\prod_{i=1}^{n} q(x_i)}^{\text{if also identically distributed}}$$

---

[2]We'll use r.v. or r.v.s (plural) as shorter notation

Given two *independent and identically distributed* (iid) random variables, one could ask how to calculate the PDF of their sum, and its characteristic function.

Assuming x_1, x_2 are two real iid random variables with PDF $q(x)$, x is their sum:

<div align="center">r.v. drawn from
↓</div>

$$x = x_1 + x_2 \qquad x_1, x_2 \sim q(x)$$

Drawing x_1, x_2 from $q(x)$, many different outcomes can add to the same sum x; these have to be added up with the corresponding probability, hence

<div align="center">because they are iids</div>

$$p(x) = \int \delta(x - (x_1 + x_2)) \overbrace{q(x_1)q(x_2)} \, dx_1 \, dx_2 \quad \equiv \quad < \delta(x - x_1 - x_2) >$$

$$= \int q(x - y)q(y) dy \tag{1.14}$$

that is a convolution of the probability density functions. The distribution of the sum of two r.v.s is the convolution of their distributions.

What is the characteristic function of $p(x)$, if the CF of $q(x)$ is $\varphi_1(k)$?

$$\varphi(k) \equiv < e^{ikx} > = \int p(x)e^{ikx} \, dx = \int dx \, e^{ikx} \delta(x - (_1 + x_2)) q(x_1)q(x_2) \, dx_1 \, dx_2$$

$$= \int e^{ik(x_1 + x_2)} q(x_1)q(x_2) \, dx_1 \, dx_2 = \int e^{ikx_1} q(x_1) \, dx_1 \int e^{ikx_2} q(x_2) \, dx_2$$

$$= \varphi_1(k)\varphi_2(k) = [\varphi_1(k)]^2 \tag{1.15}$$

Exercise 9: Exercises on sum of iid r.v.s

Calculate the distribution of $x = x_1 + x_2$ if x_1, x_2 are iids drawn from:

1. a uniform distribution $U([0, 1])$;

2. a gaussian distribution $\mathcal{N}_x(\mu, \sigma)$;

3. an exponential distribution $q(x) = \lambda e^{-\lambda x}$

Exercise 10: Exercise on product of iid r.v.s

Calculate the distribution of $x = x_1 \cdot x_2$ when x_1, x_2 are positive iid r.v.s.

Exercise 11: Exercise on sum of i r.v.s

Calculate the characteristic function of the distribution of the sum $x = x_1 + x_2 + \dots + x_n$ when x_i are independent but **not** identically distributed r.v.s.

1.4.2   The law of large numbers

Proposition 1: The (weak) law of large numbers

Given n iid random variables x_i whose PDF is $q(x_i)$, assuming that the mean of x_i is μ ($\mu = \int x_i q(x_i) \, dx_i$), defined $x = \frac{1}{n} \sum_{i=1}^{n} x_i$

$$\lim_{n \to \infty} x = \lim_{n \to \infty} \frac{1}{n} \sum_{i=1}^{n} x_i = \mu$$

This can be shown as follows, assuming $\varphi_i(k)$ to be the CF of $q(x_i)$ and $\varphi(k)$ the one of x

$$\varphi(k) \equiv < e^{ikx} > = < e^{ik\frac{1}{n}\sum_{j=1}^{n} x_j} > = \int e^{i\frac{k}{n}\sum_{j=1}^{n} x_j} q(x_1)...q(x_n) \, \mathrm{d}x_1 ... \mathrm{d}x_n$$

$$= \underbrace{\left(\int e^{i\frac{k}{n}x_1} q(x_1) \, \mathrm{d}x_1 \right)}_{\varphi_1\left(\frac{k}{n}\right)} ... \underbrace{\left(\int e^{i\frac{k}{n}x_n} q(x_n) \, \mathrm{d}x_n \right)}_{\varphi_n\left(\frac{k}{n}\right)}$$

$$= \left[\varphi_1 \left(\frac{k}{n} \right) \right]^n \tag{1.16}$$

Also,

$$\varphi_1 \left(\frac{k}{n} \right) \equiv \int e^{i\frac{k}{n}x} q(x) \, \mathrm{d}x \overset{\overset{\text{Taylor expansion of } e^x \text{ for } n >> 1}{\downarrow}}{=} 1 + \frac{ik}{n} < x > + o\left(\frac{1}{n} \right) \qquad \text{as } n \to \infty$$

Combined with equation 1.16

$$\varphi(k) = \left(1 + \frac{ik}{n}\mu + o\left(\frac{1}{n} \right) \right)^n \xrightarrow[n\to\infty]{} e^{i\mu k} = \int \underbrace{\delta(x - \mu)}_{p(x)} e^{ikx} \, \mathrm{d}x$$

This is a weak result, proving only a convergence in distribution (or in law): $\varphi(k) \to e^{i\mu k}$, showing that the CF of the empirical average converges to the CF of a Dirac delta of the true mean[3].

There is also a stronger result, which won't be proven here[4]:

Proposition 2: The (strong) law of large numbers

Let $x_1, x_2, ...x_n$ be a sequence of iid random variables each with finite mean μ. Then the finite (empirical) average approaches μ as $n \to \infty$.

$$\frac{1}{n}\sum_{i=1}^{n} x_i \underset{n}{\to} \mu \tag{1.17}$$

The law says that, for large n, the sum $\sum_{i=1}^{n} x_i$ is approximately $n\mu$. The next step is to understand how the fluctuations behave around $n\mu$, studying $\sum_{i=1}^{n} x_i - n\mu$.

1.4.3 Differences in convergence

In probability theory more than one type of convergences are defined. From the least to the most "strong":

1. convergence in distribution

2. convergence in probability

3. mean-square convergence

4. almost sure convergence

the least being the most accurate and every type of convergence implies the previous ones.

---

[3]This calculations can be found in [1] at page 199.
[4]This result is better shown in [1] at page 329.

> **Definition 5: Convergence in probability**
>
> A sequence of random variables $\{x_i\}_{i=1...n}$ converges in probability to a random variable x if
> $$\forall \epsilon > 0, \ \lim_{n \to \infty} p(|x_n - x| > \epsilon) = 0$$

where the main idea is that the probability that x_n deviate from x by more than any $\epsilon > 0$ goes to 0 as n goes to infinity. This does not guarantee that x_n goes to x as $x \to \infty$.

> **Definition 6: Almost sure convergence**
>
> A sequence of random variables $\{x_i\}_{i=1...n}$ converges almost sure to a random variable x if
> $$p \left(\lim_{n \to \infty} x_n = x \right) = 1$$
> and can be written as $\lim_{n \to \infty} x_n = x$

so for almost all realization of x_n, x_n goes to x.

> **Example 3: Differences in convergence for Bernoulli random variables**
>
> et $x_1, ..., x_n$ be Bernoulli r.v. defined as
> $$x_n = \begin{cases} 1 & p_n \\ 0 & 1 - p_n \end{cases} \qquad p_n = \frac{1}{n} \xrightarrow{n \to \infty} 0$$
>
> A realization of this sequence is a sequence of 0s and 1s, with 1s becoming rarer as $n \to \infty$, but always present (waiting enough). In this case there is convergence in probability but not almost sure convergence $(p(x_n = 1) \xrightarrow{n \to \infty} 0)$.
> In contrast, almost sure convergence is equivalent to say $\exists N$ (that depends on the specific realization of the sequence) such that $\forall n > N$, $x_n = 0$.
> In the second case the 1s should completely go extinct for $n > N$. In this example, however, convergence is only in probability, not almost sure, because as $p_n > 0$ it will be always possible to find a "1" in the sequence for n large enough.
> Using the II Borel-Cantelli Lemma it is for example possible to prove that with an initial probability $p_n = \frac{1}{n}$ it is always $(p = 1)$ possible to find an event $\{x_n = 1\}$.

As a conclusion, it is important to remember that *the weak law of large numbers* is the most general result, giving a convergence only in distribution; on the other side, *the strong law of large numbers* is a more precise and strong result, able to demonstrate an almost-sure convergence; the almost-sure convergence implies the convergence in distribution, but not the other way around.

1.4.4 Central limit theorem

There is an extraordinary result for the fluctuations, which is valid under the assumption of a finite variance for x_i:

1. $\sum_i^n x_i - n\mu$ is about as big as $\sqrt{n}$

2. The distribution of $\frac{\sum_{i=1}^n x_i - n\mu}{\sqrt{n}}$ approaches a gaussian PDF as $n \to \infty$ IRRESPECTIVE of the PDF of x

Claims 1. and 2. are the core meaning of the

Proposition 3: Central Limit Theorem

Let $x_1, ..., x_n$ be a sequence of iid r.v.s with finite mean μ and finite (non-zero) variance σ^2. Then the PDF of the fluctuations converges to a gaussian PDF with mean 0 and variance 1.

$$Y_n = \frac{\sum_{i=1}^{n} x_i - n\mu}{\sqrt{n}\sigma} \xrightarrow[n\to\infty]{} \mathcal{N}(0,1) \tag{1.18}$$

We can make some observations:

$$< Y_n > = \frac{1}{\sqrt{n}\sigma}\left(\sum_{i=1}^{n} < x_i > -\mu n\right) = 0$$

$$Var(Y_n) = \frac{1}{n\sigma^2}Var\left(\sum_{i=1}^{n} x_i - \mu n\right) = \frac{1}{n\sigma^2}Var\left(\sum_{i=1}^{n} x_i\right) = \frac{\sum_{i=1}^{n} Var(x_i)}{n\sigma^2} = \frac{n\sigma^2}{n\sigma^2} = 1$$

(the reader should go through all the steps and revise the properties of Var(...)).
This means that Y_n has a center (0) and a "width" that does not change as n varies. This theorem can be proven using the properties of the CF Assuming that each r.v. has a PDF $q(x)$ with CF $\varphi_1(k)$,

$$\varphi(k) \equiv < e^{ikY_n} > = \int e^{ik\frac{\sum_i x_i - \mu n}{\sqrt{n}\sigma}} q(x_1)...q(x_n)\,\mathrm{d}x_1 ... \mathrm{d}x_n$$

$$= e^{-\frac{ik\mu\sqrt{n}}{\sigma}}\underbrace{\left(\int e^{i\frac{k}{\sqrt{n}\sigma}x}q(x)\,\mathrm{d}x\right)^n}_{\varphi_1\left(\frac{k}{\sqrt{n}\sigma}\right)} \tag{1.19}$$

As seen in the previous theorem, as $n \to \infty$

$$\varphi_1\left(\frac{k}{\sqrt{n}\sigma}\right) \overset{\overset{\text{Taylor}}{\downarrow}}{=} 1 + \frac{ik}{\sqrt{n}\sigma}\underbrace{< x >}_{=\mu} - \frac{k^2}{2n\sigma^2}\underbrace{< x^2 >}_{=\sigma^2+\mu^2} + \mathcal{O}\left(n^{-\frac{3}{4}}\right)$$

$$= e^{\frac{ik}{\sqrt{n}\sigma}\mu - \frac{k^2}{2n}}$$

Exercise 12

Show why only $-\frac{k^2}{2n}$ remains for the exponent.

From equation 1.19

$$\varphi(k) = e^{-\frac{ik\mu}{\sigma}\sqrt{n}}e^{\frac{ik\mu}{\sigma}\sqrt{n} - \frac{k^2}{2}} = e^{-\frac{k^2}{2}}$$

that doesn't depend on n. As shown in equation 1.6, this is the CF of $p(x) = \frac{1}{\sqrt{2\pi}}e^{-\frac{x^2}{2}} \equiv \mathcal{N}(0,1)$.

Exercise 13: Exercises on Central Limit Theorem

Show that

1. $\sum_{i=1}^{n} x_i \sim \mathcal{N}(n\mu, n\sigma^2)$;

2. $\frac{1}{n}\sum_{i=1}^{n}x_i \sim \mathcal{N}(\mu, \frac{\sigma^2}{n})$

2. $\frac{1}{n}\sum_{i=1}^{n}x_i \sim \mathcal{N}(\mu, \frac{\sigma^2}{n})$

1.5   The Laplace method

In many situations, one needs to evaluate complicated integrals of the form

$$I(\lambda) = \int_{x_1}^{x_2} g(x)e^{\lambda f(x)} \, \mathrm{d}x \qquad \lambda \in \mathbb{R} \tag{1.20}$$

Although $I(\lambda)$ cannot be calculated for an arbitrary λ, it can be well approximated as $\lambda \to \infty$. Let's assume that f and g are continuous, differentiable real-valued functions in the interval $[x_1, x_1]$. In particular, a consequence of Weierstrass theorem, $f(x_0)$ has global extrema in $[x_1, x_2]$. We are interested in its point(s) of global maximum: let's assume that there exists only one[5] of such points, say x_0. Also, let's assume that $f''(x_0) \neq 0$ and that $g(x_0) \neq 0$. The main idea of Laplace's method is that, for $\lambda \to +\infty$, the leading contribution to the integral will come from the exponential term $e^{\lambda f(x)}$. Specifically, it will come from the neighborhood of x_0, since the ratio

$$\frac{g(x) \cdot e^{\lambda f(x)}}{g(x_0) \cdot e^{\lambda f(x_0)}} \simeq 1 \cdot e^{-\lambda \cdot |f(x_0) - f(x)|}$$

becomes vanishingly small when $\lambda \to +\infty$ (see Fig. 1.1).
There are essentially 3 cases:

1. x_0 is an *internal maximum point*: $x_0 \in]x_1, x_2[$

2. x_0 is a *flat endpoint maximum*: $x_0 = x_1$ (or $x_0 = x_2$) and $f'(x_0) = 0$

3. x_0 is a *not flat endpoint maximum*: $x_0 = x_2$ (or $x_0 = x_2$) and $f'(x_0) \neq 0$

1.5.1   Internal maximum: $x_0 \in]x_1, x_2[$

In this case the maximum x_0 of (x) is interior to the interval $[x_1, x_2]$ $(x_0 \in (x_1, x_2))$ and $f'(x_0) = 0$. Working with the maximum condition in x_0 it is possible to assume $f''(x_0) < 0$ (it is not more different assuming $f^i(x_0) = f^{ii}(x_0) = f^{iii}(x_0) = 0$ and $f^{iv}(x_0) < 0$ or equivalent for any even derivative), $g(x_0) \neq 0$ and finite (otherwise the maximum condition for $f(x)$ wouldn't be relevant for $I(\lambda)$). With those conditions, $f(x)$ is smooth up to the second order in $[x_1, x_2]$ (continuously differentiable). The dominant part comes from the neighborhood of x_0 and using

---

[5]the case in which the maximum is attained in two ore more points can be addressed the same way: say $a \leq x_0 < x_1 \leq b$ are two points of global maximum, then one can split $I(\lambda)$ as $I(\lambda) = \int_a^{x_1 - \delta} g(x)e^{\lambda f(x)} \, \mathrm{d}x + \int_{x_1 + \delta}^b g(x)e^{\lambda f(x)} \, \mathrm{d}x$
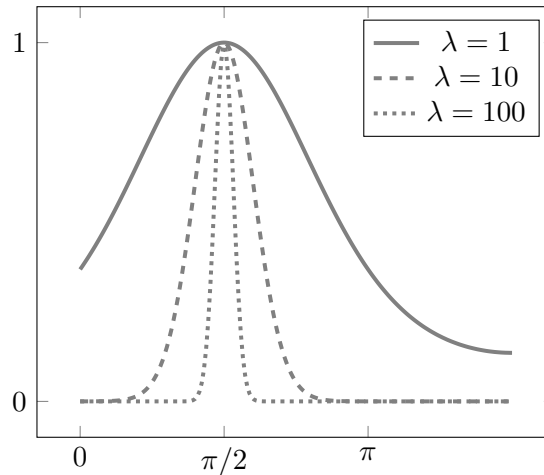

Fig. 1.1: The function $e^{\lambda(sin(x)-1)}$ for increasing values of λ.

Taylor expansion $f(x) = f(x_0) + \frac{(x-x_0)2}{2}f''(x_0) + o(|x - x_0|^2)$ as $x \to x_0$; introducing the expansion in $I(\lambda)$ the result is the approximation

$$I(\lambda) \simeq \int_{x_1}^{x_2} g(x)e^{\lambda\left(f(x_0)+\frac{(x-x_0)^2}{2}f''(x_0)\right)}\,\mathrm{d}x = g(x_0)e^{\lambda f(x_0)}\int_{x_1}^{x_2}e^{-\lambda\frac{(x-x_0)^2}{2}|f''(x_0)|}\,\mathrm{d}x$$

changing variable to: $s = (x - x_0)\sqrt{\frac{|f''(x_0)|}{2}\lambda}$

$$I(\lambda) \simeq g(x_0)e^{\lambda f(x_0)}\sqrt{\frac{2}{\lambda\,|f''(x_0)|}}\int_{s_1}^{s_2}e^{-s^2}\,\mathrm{d}s \xrightarrow{\lambda\to\infty} \int_{-\infty}^{+\infty}e^{-s^2}\,\mathrm{d}s = \sqrt{\pi}$$

$$\text{as}\quad s_1 = (x_1 - x_0)\sqrt{\frac{|f''(x_0)|}{2}\lambda} \xrightarrow{\lambda\to\infty} -\infty \quad s_2 = (x_2 - x_0)\sqrt{\frac{|f''(x_0)|}{2}\lambda} \xrightarrow{\lambda\to\infty} +\infty$$

obtaining the *leading order* approximation:

$$I(\lambda) \simeq g(x_0)e^{\lambda f(x_0)}\sqrt{\frac{2\pi}{\lambda\,|f''(x_0)|}} \qquad as\ \lambda \to +\infty \qquad\qquad (1.21)$$

Exercise 14: Better Laplace method approximation

Show that a better approximation is given by

$$I(\lambda) \simeq e^{\lambda f(x_0)}\sqrt{\frac{2\pi}{\lambda\,|f''(x_0)|}}\left(g(x_0) + \frac{c}{\lambda}\right) \qquad as\ \lambda \to +\infty$$

where c is a constant that depends on derivatives of $f(x)$ up to 4th order (at $x = x_0$) and on $g(x_0)$, $g'(x_0)$ and $g''(x_0)$.

1.5.2   Flat endpoint maximum: $x_0 = x_1$ or $x_0 = x_2$ with $f'(x) = 0$

In this case, x_0 is an endpoint and a maximum for $f(x)$, $f'(x_0) = 0$ and $f''(x_0) < 0$ as in the previous case. Following the same steps as before:

$$I(\lambda) \simeq \int_{x_1}^{x_2} g(x)e^{\lambda\left(f(x_0)+\frac{(x-x_0)^2}{2}f''(x_0)\right)}\,\mathrm{d}x = g(x_0)e^{\lambda f(x_0)}\int_{x_1}^{x_2}e^{-\lambda\frac{(x-x_0)^2}{2}|f''(x_0)|}\,\mathrm{d}x$$

$$= g(x_0)e^{\lambda f(x_0)}\sqrt{\frac{2}{\lambda\,|f''(x_0)|}}\int_{0}^{s_2}e^{-s^2}\,\mathrm{d}s \xrightarrow{\lambda\to\infty} \int_{0}^{+\infty}e^{-s^2}\,\mathrm{d}s = \frac{\sqrt{\pi}}{2}$$

$$\text{as}\quad s_1 = (x_1 - x_0)\sqrt{\frac{|f''(x_0)|}{2}\lambda} = 0 \text{ for } x_0 = x_1 \quad s_2 = (x_2 - x_0)\sqrt{\frac{|f''(x_0)|}{2}\lambda} \xrightarrow{\lambda\to\infty} +\infty$$

obtaining the *leading order* approximation:

$$I(\lambda) \simeq g(x_0)e^{\lambda f(x_0)}\sqrt{\frac{\pi}{2\lambda\,|f''(x_0)|}} \qquad as\ \lambda \to +\infty \qquad\qquad (1.22)$$

The Laplace method is one of the most used methods to study special functions in large parameter regimes, like in the next example.

Example 4: Modified Bessel function

he modified Bessel function of the second kind is a special function that occurs in many applications. There exist an integral representation:

$$k_\nu(x) = \int_0^\infty e^{-x\cosh(t)}\cosh(\nu t)\,\mathrm{d}t$$

One can wish to estimate $k_\nu(x)$ as $x \to +\infty$ for fixed ν.

Since the derivative $\cosh'(t)0\sinh(t)$ is positive for $t > 0$, the max of $e^{-x\cosh(t)}$ as a function of t (for fixed $x > 0$) occurs at $t = 0$ (the left edge). Equation 1.22 can then be applied

$$\cosh(t) \simeq 1 + \frac{t^2}{2} + \text{h.o.t.}$$

$$k_\nu(x) \simeq e^{-x}\sqrt{\frac{\pi}{2x}} \quad \text{leading order at } x \to \infty$$

NOTE: it does not depend on ν!

Exercise 15: Better modified Bessel function approximation

Show that a better approximation is given by

$$k_\nu(x) \simeq e^{-x}\sqrt{\frac{\pi}{2x}}\left(1 + \frac{c(\nu)}{x}\right) \qquad as\ \lambda \to +\infty$$

and calculate $c(\nu) = \frac{4\nu^2 - 1}{8}$.

1.5.3 Non flat endpoint maximum: $x_0 = x_1$ or $x_0 = x_2$ but $f'(x) \neq 0$

In this case, x_0 is an endpoint but not a relative maximum for $f(x)$, $f'(x_0) \neq 0$. Without loss of generality, it is possible to choose $x_0 = x_1$ and $f'(x_0) < 0$ (or the analogous $x_0 = x_2$ and $f'(x_0) > 0$, because $f(x)$ needs to assume the maximum value in x_0). Then

$$f(x) = f(x_0) + (x - x_0)f'(x_0) + \text{h.o.t.}$$

$$I(\lambda) \simeq \int_{x_1=x_0}^{x_2} g(x)e^{\lambda[f(x_0)+(x-x_0)f'(x_0)]}\,\mathrm{d}x \ \simeq\ g(x_0)e^{\lambda f(x_0)}\int_{x_1=x_0}^{x_2} e^{\lambda(x-x_0)f'(x_0)}\,\mathrm{d}x$$

$$\text{for } s = x - x_0: \ = g(x_0)e^{\lambda f(x_0)}\int_0^{x_2-x_1} e^{\lambda s f'(x_0)}\,\mathrm{d}s \ = \ \frac{g(x_0)e^{\lambda f(x_0)}}{\lambda f'(x_0)}\left[e^{\lambda s f'(x_0)}\right]_0^{x_2-x_1}$$

$$= \frac{g(x_0)e^{\lambda f(x_0)}}{\lambda f'(x_0)}\left(e^{\lambda(x_2-x_1)f'(x_0)} - 1\right) \ \xrightarrow{\lambda\to\infty}\ -\frac{g(x_0)e^{\lambda f(x_0)}}{\lambda f'(x_0)}$$

recalling that $f'(x_0) < 0$ and with exponentially small terms; this result can be written in a synthetic form to comprehend both endpoint cases as

$$I(\lambda) \simeq g(x_0)\frac{e^{\lambda f(x_0)}}{\lambda\,|f'(x_0)|} \qquad \text{as } \lambda \to \infty \tag{1.23}$$

To summarize, *Laplace method* can be used for integrals with an **exponential form** where the parameter (λ) that goes to infinity is *only* present at the exponent; in this case, if a maximum for the function is present *in* the integration interval, the **leading order** is $\propto \frac{e^\lambda}{\sqrt{\lambda}}$, otherwise for an edge point that is not a flex maximum, the **leading order** is $\propto \frac{e^\lambda}{\lambda}$.

Note that the exponential form of the integral is necessary to guarantee that the excluded terms are negligible. Multiple maxima in $[x_1 x_2]$ with equal value can be dealt with similarity.

Example 5: End point maximum

We can obtain the leading order approximation of the following applying equation 1.23

$$I(\lambda) = \int_0^1 x^m e^{\lambda\left(3x^2 + 2x^3\right)} \, dx \simeq \frac{e^{5\lambda}}{12\lambda} \qquad \text{as } \lambda \to \infty, \text{ fixed } m$$

where the max is at $x = 1$ with $f(1) = 5$, $f'(1) = 12$, $g(1) = 1$. Observe the absence of dependence on m.

It is possible to understand how fast $N!$ goes to infinity as N grows applying Laplace's method to the gamma function, which is defined as

$$\Gamma(\lambda) \equiv \int_0^\infty x^{\lambda-1} e^{-x} \, dx \qquad Re(\lambda) > 0 \tag{1.24}$$

Exercise 16: Demonstration of Gamma function and factorial relation

Show that $\Gamma(\lambda+1) = \lambda\Gamma(\lambda)$, hence $\lambda! = \Gamma(\lambda+1)$ which generalize the factorial to real (and complex) numbers.

Using for the function $\Gamma(\lambda+1) = \int_0^\infty x^\lambda e^{-x} \, dx$ an equivalent form $\Gamma(\lambda+1) = \int_0^\infty e^{\lambda \ln(x)} e^{-x} \, dx$ the Laplace method cannot be applied directly. In fact, using the previous formalism, $f(x) = -x + \lambda \ln(x)$ and $g(x) = 1$, and the maximum occurs at $x = \lambda$, resulting in a movable maximum for variation of λ. The maximum itself suggests a change of variable to bypass the problem: $x = \lambda t$; as further shown this allows the maximum to be fixed, no longer depending on λ:

$$\Gamma(\lambda+1) = \int_0^\infty x^\lambda e^{-x} \, dx \overset{\overset{x = \lambda t}{\downarrow}}{=} \lambda^{\lambda+1} \int_0^\infty t^\lambda e^{-\lambda t} \, dt$$

$$t^\lambda e^{-\lambda t} = e^{\lambda(\ln(t) - t)}$$

$$h(t) = \ln(t) - t, \qquad\qquad\qquad h(t) = 0 \text{ for } t = 1$$

$$h'(t) = \frac{1}{t} - 1 \qquad\qquad\qquad h'(1) = 0$$

$$h''(t) = \frac{-1}{t^2} \qquad\qquad\qquad h''(1) = -1$$

it is now possible to apply equation 1.21 for $g(t) = 1$ and $t_0 = 1$

$$\Gamma(\lambda+1) = \lambda! \simeq \lambda^{\lambda+1} e^{-\lambda} \sqrt{\frac{2\pi}{\lambda}} \qquad \text{as } \lambda \to +\infty \tag{1.25}$$

which is the Stirling's formula. It is possible to improve it with a factor $\left(1 + \frac{1}{12\lambda}\right)$.

Exercise 17

Verify the following for large λ

1. $I(\lambda) = \int_0^\infty e^{-\lambda t} e^{-\frac{1}{t}} \, dt \simeq \dfrac{\sqrt{\pi} e^{-2\sqrt{\lambda}}}{\lambda^{\frac{3}{4}}}$ (Application of Stirling's Formula)

2. $I(\lambda) = \int_{-2}^0 e^t e^{\lambda(3t^2+2t^3)} \, dt \approx e^{\lambda-1}\sqrt{\dfrac{\pi}{3\lambda}}$

3. $I(\lambda) = \int_0^1 e^t e^{\lambda(3t^2+2t^3)} \, dt \approx e^{5\lambda+1}\dfrac{1}{12\lambda}$

4. $I(\lambda) = \int_0^1 \sqrt{t+1}\, e^{\lambda(2t-t^2)} \, dt \approx e^{\lambda}\sqrt{\dfrac{\pi}{2\lambda}}$

5. $I(\lambda) = \int_{-2}^0 (1+t^2) e^{\lambda(t^3-1)} \, dt \approx 5e^{6\lambda}\dfrac{1}{12\lambda}$

1.5.4 Lp norm in real analysis

The quantity

$$||g||_p := \left(\int_a^b |g(t)|^p \, dt \right)^{\frac{1}{p}}$$

is known as Lp-norm in real analysis. The integral exists in Lebesgue sense. One can be interested in the behavior of $||g||_p$ as $p \to \infty$ when g has a unique absolute maximum at the internal point t_0 and $g \in C^4(a,b)$. It is useful to study first

$$I(p) = \int_a^b |g(t)|^p \, dt \qquad ||g||_p = I(p)^{\frac{1}{p}}$$

so that

$$I(p) = \int_a^b e^{p\ln|g(t)|} \, dt$$

An assumption that was made formulating the Laplace method is that $f(x)$, the function at the exponential, has to be continuously differentiable in $[a,b]$. In this case, if g vanishes somewhere in $[a,b]$, then $\ln|g(t)| \to -\infty$. However every neighborhood of points where $g = 0$ will yield a negligible contribution to $I(p)$ for large p. Thus such discontinuities can be neglected. Equation 1.21 can thus be applied with $g(t) = 1$

$$I(p) = e^{p\ln|g(t_0)|}\sqrt{\dfrac{2\pi\,|g(t_0)|}{p\,|g''(t_0)|}}\left(1 + \mathcal{O}\left(\dfrac{1}{p}\right)\right)$$

$$= |g(t_0)|^p \sqrt{\dfrac{2\pi\,|g(t_0)|}{p\,|g''(t_0)|}}\left(1 + \mathcal{O}\left(\dfrac{1}{p}\right)\right) \qquad \text{as } p \to +\infty$$

Since $\quad a^{\frac{1}{p}} p^{-\frac{1}{2p}} = e^{\frac{\ln a}{p}} e^{-\frac{\ln p}{2p}} \simeq \left(1 + \dfrac{\ln a}{p} + ...\right)\left(1 - \dfrac{\ln p}{2p} + ...\right) \simeq 1 - \dfrac{\ln p}{2p} + h.o.t.$

$$I(p)^{\frac{1}{p}} = |g(t_0)|\left(\dfrac{2\pi\,|g(t_0)|}{p\,|g''(t_0)|}\right)^{\frac{1}{2p}} + h.o.t. = |g(t_0)|\left(1 - \dfrac{\ln p}{2p} + \mathcal{O}\left(\dfrac{1}{p}\right)\right) \qquad \text{as } p \to +\infty$$

hence $\quad ||g||_p = |g(t_0)| t \in [a,b]\left\{1 - \dfrac{\ln p}{2p} + \mathcal{O}\left(\dfrac{1}{p}\right)\right\} \qquad \text{as } p \to +\infty.$

Example 6: Multiples maxima in range

Consider the integral

$$I(\lambda) = \int_0^{\frac{3\pi}{2}} e^{-\lambda \sin(t)} f(t) \, dt$$

where $f(x)$ is continuously differentiable in $[0; \frac{3\pi}{2}]$. The contributions from the endpoint minima $t = 0$ and $t = \frac{3\pi}{2}$ must both be considered.

$$I(\lambda) = \underbrace{\int_0^{\frac{\pi}{2}} e^{-\lambda \sin(t)} f(t) \, dt}_{I_1} + e^{\lambda} \underbrace{\int_{\frac{\pi}{2}}^{\frac{3\pi}{2}} e^{-\lambda \sin(t)\lambda} f(t) \, dt}_{I_2}$$

applying now equation 1.22

$$I_1(\lambda) = f(0) \frac{e^{\lambda \cdot 0}}{\lambda |\cos(0)|} \simeq \frac{f(0)}{\lambda} \qquad \text{as } \lambda \to +\infty$$

$$I_2(\lambda) = f\left(\frac{3\pi}{2}\right) e^{\lambda \cdot 0} \sqrt{\frac{\pi}{2\lambda |\sin(\frac{3\pi}{2})|}} = f\left(\frac{3\pi}{2}\right) \sqrt{\frac{\pi}{2\lambda}} \qquad \text{as } \lambda \to +\infty$$

hence the leading contribution comes from I_2 and

$$I(\lambda) \simeq f\left(\frac{3\pi}{2}\right) e^{\lambda} \sqrt{\frac{\pi}{2\lambda}} + h.o.t. \qquad \text{as } \lambda \to +\infty$$

The minimum at t=0 is subleading and should be taken into account only at higher order.

Example 7: Movable maximum for a class of functions

Consider the class of integrals

$$I_m(x) = \int_0^{\infty} t^m e^{-\frac{t^2}{2} - \frac{x}{t}} \, dt \qquad x > 0$$

where is asked to evaluate $I_m(x)$ as $x \to +\infty$ with fixed m. The function $\frac{t^2}{2} + \frac{x}{t}$ has a movable minimum at

$$\frac{d}{dt}\left(\frac{t^2}{2} + \frac{x}{t}\right) = t - \frac{x}{t^2} = 0, \qquad \bar{t} = x^{\frac{1}{3}}$$

it proves useful to change the variable, in order to fix the minimum, as

$$t = x^{\frac{1}{3}} \tau$$

So $I_m(x)$ can be recast in the form

$$I_m(x) = x^{\frac{m+1}{3}} \int_0^{\infty} \tau^m e^{-x^{2/3}\left(\frac{\tau^2}{2} + \frac{1}{\tau}\right)} \, d\tau$$

for minimum of $\left(\frac{\tau^2}{2} + \frac{1}{\tau}\right)$ occurs at $\tau = 1$ (interior of the interval), so the equation 1.21 can be applied

$$I_m(x) \simeq x^{\frac{m+1}{3}} e^{-\frac{3}{2}x^{2/3}} \sqrt{\frac{2\pi}{x^{\frac{2}{3}} \cdot 3}} \qquad \text{as } x \to +\infty$$

$$= x^{\frac{m}{3}} e^{-\frac{3}{2}x^{2/3}} \sqrt{\frac{2\pi}{3}}$$

at leading order in x with fixed m.

Chapter 2

Deterministic Reaction Dynamics

Chemical reaction form a broad field of applications where deterministic and stochastic methods are very useful. The term reaction is used here in a very general form. Although the terminology is directly taken from chemistry, referring to **reactants** and **products**, the framework developed in this chapter could be used to model a wide class of systems. Such reactions include any system or process that involves individuals of the same or different species randomly encountering each others (**reactants**) and transforming, producing individuals (**products**) which may be of a different nature with relation to the reactants. Examples of systems that can be studied within this framework include, but are not limited to:

- Actual **chemical reactions**, which involve particles or molecules that transform upon collisions;

- **Population systems**, where individuals may die, reproduce, consume other individuals, immigrate, etcetera;

- **Epidemics**, which involve the transmission of a desease to individuals that might be susceptible, infected, cured;

- **Gene expression**, where genes can be transcripted (into mRNA) and translated (into proteins) upon the appropriate occurance of some transcription factors.

In this chapter the focus will be on deterministic methods, without considering the stochastic properties of these systems. These deterministic models can always be thought as the mean field approaches to the corresponding problem.

2.1 Binary irreversible reactions

Let's start by considering a simple bynary irreversible reaction in which two species X and Y are consumed to produce Z. A reaction is **reversible** if it can occur in the backward direction, so if the products upon collision can react to give the reactants. In this first example the backward reaction is not possible. Using the usual representation of chemical reaction we would write

$$X + Y \xrightarrow{k} Z \tag{2.1}$$

Note however that a more general reaction might involve the consumption or production of more that one individual of some species. For example in the well know reaction

$$2H_2 + O_2 \xrightarrow{k} 2H_2O$$
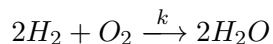
2 molecules of hydrogen are consumed and 2 of water are produced. These coefficients, definig the number of individuals involved in the reaction, are called **stoichiometric coefficients**.

2.1.1   Calculation of the reaction rates

Assuming that the reaction occurs in a **finite** volume V (non necessarily a physical volume, but some finite environment whose dimensions are grater than the reactants' characteristic length) where the **individuals** (molecules, ...) are **well-stirred/mixed** and the concentration of the species X, Y, Z are "**small**", despite the number of individuals of each type is "**large**", it is possible to assume that the **interaction** between individuals are **random** and that **crowding effects** can be ignored. This is called **diluted limit**, and allows also the assumption of **continuous variables** for the concentrations of the individuals:

$$x = \frac{n_x}{V} , \quad y = \frac{n_y}{V} , \quad z = \frac{n_z}{V} , \quad (n_i : \text{number of individuals of type I})$$

Going back to (2.1), it is possible to estimate $r(x, y)$, the **reaction rate**, in the **diluted limit**:

$$r(x, y) \simeq r(0, 0) + \left(\frac{\partial r}{\partial x}\right)(0, 0)x + \left(\frac{\partial r}{\partial y}\right)(0, 0)y+ \tag{2.2}$$

$$+ \frac{1}{2}\left(\frac{\partial^2 r}{\partial x^2}\right)(0, 0)x^2 + \frac{1}{2}\left(\frac{\partial^2 r}{\partial y^2}\right)(0, 0)y^2 + \left(\frac{\partial^2 r}{\partial x \partial y}\right)(0, 0)xy + h.o.t.$$

However, since for the reaction to occur both reactants X and Y are required:

$$r(x, 0) = r(0, y) = 0 \qquad \forall x, y$$

which must be considered identities, defining what a reaction is (without one of the reactants the reaction should not occur). Using a Taylor expansion also for these terms:

$$r(x, 0) = r(0, 0) + (\partial_x r_0)\, x + \left(\frac{1}{2}\partial_{xx}^2 r_0\right) x^2 = 0$$

$$r(0, y) = r(0, 0) + (\partial_y r_0)\, y + \left(\frac{1}{2}\partial_{yy}^2 r_0\right) y^2 = 0$$

and combining them with eq. (2.2) gives

$$r(x, y) \approx \left(\frac{\partial^2 r}{\partial x \partial y}\right)(0, 0)xy \equiv kxy \tag{2.3}$$

where k is called **kinetic constant** of the reaction.

Fundamental Observation: in this approximation particles (or individuals) are free to move around and randomly meet each others: the probability of X and Y to collide are **independent**. When they meet, they react (for now, with probability $p = 1$). This is the basic diluted limit hypothesis, in this case the kinetic constant does not depend on concentrations; however k may depend on the temperature by the mean of the Arrhenius factor $e^{-\frac{E}{kT}}$, so that $k = k_0 e^{-\frac{E}{kT}}$, for E activation energy. Generalizations can be easily made, including a differnt probability for the reaction to occur, or a dependence of k on the concentrations, BUT the kinetic constant must be always strictly positive.

The assumptions and considerations that lead to the previous result are usually enounced as an approximate/empirical "law", simple and useful in many situations:

Proposition 4: The Law of Mass Action

In a first approximation, the rate of any chemical reaction is proportional to the product of the concentrations of the reacting substances.

This law can be used to deduce the ODEs for the time evolution of the concentrations. If the concentrations at time t is known, then at time $t + \Delta t$ using equation (2.1) they can be expressed as:

$$
\begin{matrix}
x(t + \Delta t) = x(t) - k\, x(t)\, y(t)\, \Delta t \\
y(t + \Delta t) = y(t) - k\, x(t)\, y(t)\, \Delta t \\
z(t + \Delta t) = z(t) + k\, x(t)\, y(t)\, \Delta t
\end{matrix}
\quad \xrightarrow{\Delta t \to 0} \quad
\begin{cases}
\dot{x} = -kxy, & x(0) = x_0 \\
\dot{y} = -kxy, & y(0) = y_0 \\
\dot{z} = kxy, & z(0) = z_0
\end{cases}
\tag{2.4}
$$

The logistic equation

Observe that from 2.4 come a copule of *conservation laws*:

$$\dot{x} - \dot{y} = 0$$
$$\dot{x} + \dot{z} = 0$$

therefore

$$x(t) - y(t) = x_0 - y_0 =: c$$
$$x(t) + z(t) = x_0 + z_0$$

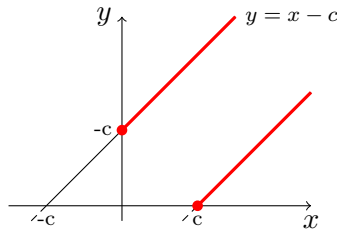that can be represented into the graph 2.1 and 2.2 respectively.

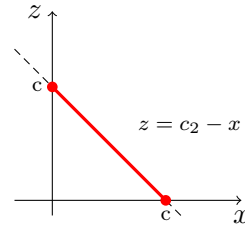**Fig. 2.1:** Graph of the evolutions of x and y: at different times it moves on a straight line

Fig. 2.2: Graph of the evolutions of x and z: $z = -x + c$

The conservation laws deduced above can be used to simplify 2.4: the equation for x becomes

$$\dot{x} = -k\,x\,y = -k\,x(x - c)$$
$$\dot{x} = k\,x(c - x) \tag{2.5}$$

the so called **logistic equation**, which can be integrated by separation of variables. For $c \neq 0$:

$$\dot{x} = \frac{\mathrm{d}x}{\mathrm{d}t} = k\,x(c - x) \qquad \frac{\mathrm{d}x}{x(c - x)} = k\,\mathrm{d}t$$

$$\int \left(\frac{A}{x} + \frac{B}{c - x} \right) \mathrm{d}x = \int k\,\mathrm{d}t \qquad \text{for } A = B = \frac{1}{c}$$

$$\frac{1}{c}\left[\ln(x) - \ln(c - x) \right] = k\,t + q \qquad \frac{x}{c - x} = e^{ckt+q}$$

$$x\left(1 + e^{ckt+q}\right) = c\,e^{ckt+q} \qquad x(t) = \frac{q\,c\,e^{ckt}}{1 + q\,e^{ckt}}$$

$$\text{for } x(0) = x_0 \quad x(0) = \frac{q\,c}{1 + q} = x_0 \qquad q = \frac{x_0}{c - x_0} \qquad \frac{x_0\,c\,e^{ckt}}{(c - x_0) + x_0\,e^{ckt}} \frac{c - x_0}{c - x_0}$$

$$x(t) = \frac{x_0 c e^{ckt}}{c + x_0(e^{ckt} - 1)} \xrightarrow{t \to +\infty} \begin{cases} c = x_0 - y_0 & \text{if } c > 0 \;\Leftrightarrow\; (x_0 > y_0) \\ 0 & \text{if } c < 0 \end{cases} \tag{2.6}$$

Observe that

- If $c > 0$, $(x_0 > y_0)$, as $t \to +\infty$, $x(t) \to c = x_0 - y_0$, $y(t) \to 0$ and $z(t) \to z_0 + y_0$;

- Conversely, if $c < 0$, $x(t) \to 0$, $y(t) \to -c = y_0 - x_0$, $x(t) \to 0$ and $z(t) \to z_0 + x_0$.

where the equations for the concentration of product Z can be found using the other independent conservation law: $\dot{x} + \dot{z} = 0 \Rightarrow x(t) + z(t) = x_0 + z_0$. In both cases the reagent having the least initial concentration is fully used up and determines the final gained amount of product.

Exercise 18: Special case: equal concentrations

Solve the logistic equation in the critical case $c = 0$. What is the interpretation in term of reagents and products?

2.2 Binary reversible reactions

Let's now consider a bynary *reversible* reaction, in which two species X and Y are consumed to produce Z and the product Z itself can react to produce the initial reactants with a different kinetic constant. The usual representation becames:

$$X + Y \underset{k_-}{\overset{k_+}{\rightleftharpoons}} Z \qquad k_\pm > 0 \tag{2.7}$$

Along the same lines as before is possible to deduce the evolution of concentrations:

$$\begin{cases} \dot{x} = +k_- z - k_+ xy, & x(0) = x_0 \\ \dot{y} = +k_- z - k_+ xy, & y(0) = y_0 \\ \dot{z} = -k_- z + k_+ xy, & z(0) = z_0 \end{cases} \tag{2.8}$$

where concentration of X increases because some Z becomes X, but also decreases because it reacts with Y to produce Z: it is equivalent to the system obtained coupling the reactions $X + Y \overset{k_+}{\longrightarrow} Z$ and $Z \overset{k_-}{\longrightarrow} X + Y$.

As before, two independent conservation laws can be verified:

$$\dot{x} - \dot{y} = 0 \qquad\qquad\qquad x(t) - y(t) = c_1$$
$$\dot{x} + \dot{z} = 0 \qquad\qquad\qquad x(t) + z(t) = c_2$$

Hence the equation for x can be written as:

$$\dot{x} = k_+ x(c_1 - x) + k_-(c_2 - x) \tag{2.9}$$

Exercise 19: Solution of the reversible equation for X

Observation: this equation (2.9) can also be solved analitically. Do it.

Example 8: Stationary concentrations form initial concentrations

Find the Stationary concentrations of the reaction in equation (2.7), when the initial concentrations are x_0, y_0, z_0.
From equation (2.8) $\dot{x} = k_- z - k_+ x y$; imposing the stability condition $\dot{x} = 0$

$$\dot{x} = 0 \Rightarrow \frac{\bar{x}\,\bar{y}}{\bar{z}} = \frac{k_-}{k_+} \quad \text{for } \bar{x}, \bar{y}, \bar{z} \text{ stationary concentrations}$$

using the concentration laws $x(t) - y(t) = c_1 = x(0) - y(0)$ and $x(t) + z(t) = c_2 = x(0) + z(0)$,
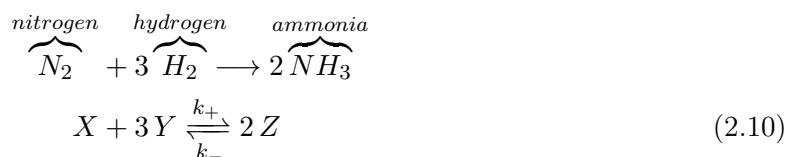
$$\frac{\bar{x}\,\bar{y}}{\bar{z}} = \frac{\bar{x}(\bar{x} - x_0 + y_0)}{x_0 + z_0 - \bar{x}} = \frac{k_-}{k_+}$$

$$\text{Hence,} \quad \bar{x}^2 + \left(y_0 - x_0 + \frac{k_-}{k_+}\right)\bar{x} - \frac{k_-}{k_+}(x_0 + z_0) = 0$$

where the *positive solutions* will be taken and then substituted into $\bar{y} = \bar{x} - x_0 + y_0$ and $\bar{z} = -\bar{x} + x_0 + z_0$.

2.2.1 The Haber process

This chemical process was developed by Fritz Haber in the early '900s and granted him the Nobel Prize in Chemistry in the year 1918. It was developed to produce ammonia on an industrial scale; apart from its historical value, it is presented here to study the role of *stoichiometric coefficients*:

$$\overbrace{N_2}^{nitrogen} + 3\,\overbrace{H_2}^{hydrogen} \longrightarrow 2\,\overbrace{NH_3}^{ammonia}$$

$$X + 3\,Y \underset{k_-}{\overset{k_+}{\rightleftharpoons}} 2\,Z \tag{2.10}$$

The corresponding ODEs for the concentrations are then:

$$\begin{cases} \dot{x} = -k_+\,x\,y^{\mathbf{3}} + k_-\,z^{\mathbf{2}} & \text{a)} \\ \dot{y} = -\mathbf{3}\,k_+\,x\,y^{\mathbf{3}} + \mathbf{3}\,k_-\,z^{\mathbf{2}} & \text{b)} \\ \dot{x} = +\mathbf{2}\,k_+\,x\,y^{\mathbf{3}} - \mathbf{2}\,k_-\,z^{\mathbf{2}} & \text{c)} \end{cases} \tag{2.11}$$

How the stoichiometric coefficients enter the ODEs:
The interpretation of the term $-3\,k_+\,x\,y^3$ in equation (2.11.b) follows from equation (2.10), in which 3 molecules (or moles) of Y have to collide indipendently along with one molecule (or mole) of X for the reaction to occur in the forward $(+)$ direction; in addiction to that, because for every molecule of X three molecules of Y reacts, for every unit decrease in concentration x, there is a threefold decrease in concentration y.
Thus, the stoichiometric coefficients affect two thing at the same time:

- the probability of a reaction to occur

- the realtive speed of the reaction as well.

The term $3k_-z^2$ has a similar interpretation: to produce Y, two molecules of Z have to collide, and this will generate 3 molecules of Y. Similarly, for every 2 molecules of Z that decompose in this way (the backward direction -) there will be 3 molecules of Y. This means that the speeds of reactions are $3\,|\dot{z}| = 2\,|\dot{y}|$. Looking at equations (2.11.b,.c) it is possible to observe that $3\dot{z} = -2\dot{y}$ because the decrease of Y leads to an increase of Z and vice versa. This is a conservation law and an analogous result can be found noticing $3\,|\dot{x}| = |\dot{y}|$, $3\dot{x} - \dot{y} = 0$.

Exercise 20: Analysis of conservation laws

Observation: at stationarity $\frac{x\,y^3}{z^2} = \frac{k_-}{k_+}$, but there are also some conservation laws:

$$3x(t) - y(t) = c_1, \qquad 2x(t) + z(t) = c_2, \qquad 2y(t) + 3z(t) = c_3$$

why are these quantities conserved and why are c_1, c_2, c_3 not independent?

2.2.2 The law of mass action (II)

With the previous considerations it is possible to restate the law of mass action as it follows

---

Proposition 5: The Law of Mass Action

In a first approximation, the rate of any chemical reaction is proportional to the product of the concentrations of the reacting substances, where every concentration is rised to a power equal to the corresponding stoichiometric coefficient, which also has to be included in the reaction speed with the appropriate sign.

The general binary reversible reaction, where a (mol) of type X react with b (mol) of type Y to obtain c (mol) of type Z and d (mol) of type W, while been reversible, is described as:

$$a\,X + b\,Y \underset{k_-}{\overset{k_+}{\rightleftharpoons}} c\,Z + d\,W \qquad a, b, c, d \in \mathbb{N} \tag{2.12}$$
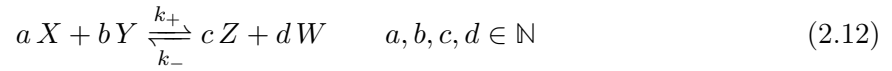
This leads to the following ODEs:

$$\begin{cases} \dot{x} = a\left(-k_+\, x^a\, y^b + k_-\, z^c\, w^d\right) \\ \dot{y} = b\left(-k_+\, x^a\, y^b + k_-\, z^c\, w^d\right) \\ \dot{z} = c\left(+k_+\, x^a\, y^b - k_-\, z^c\, w^d\right) \\ \dot{w} = d\left(+k_+\, x^a\, y^b - k_-\, z^c\, w^d\right) \end{cases}$$

these are sufficient to implement a stochastic method: with a random variable drawn from $(0; 1)$ and then composed to the probability of the reaction, it is possible to construct the system with stochastic programs, computing the stochastic evolution for time $\bar{t}$ or until the stationarity. Computing the stochastic evolution of the equation for large numbers and taking the average stochastic trajectory gives results in accord with the ODEs.

Exercise 21: General binary reversible equation analysis

Calculate the conserved quantities for the equation (2.12) using the corresponding ODEs.
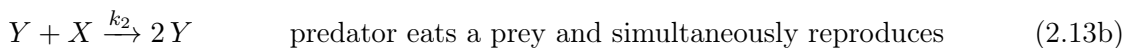

Exercise 22: Reaction rate for water

For the reversible reaction described by the well known equation, presented at the beginning of this chapter:

$$2H_2 + O_2 \underset{k_-}{\overset{k_+}{\rightleftharpoons}} 2H_2O$$
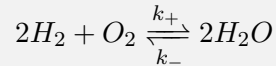
1. write down the ODEs for the rate equation

2. calculate the conservation laws and the stationary values of the concentrations starting from $x_0 = 2y_0$ and $z_0 = 0$

3. solve the final equation when $k_+ = k_-$ and $x_0 = 1$ (mol).

2.2.3   The predator and prey system

There are types of molecules or species that can interact in <u>different</u> kinds of reactions. One the most famous example is the <u>Predator and prey system</u>, where predators (Y) and preys (X) interact by means of irreversible reactions:

$$X \xrightarrow{k_1} 2\,X \qquad\qquad \text{reproduction of preys: any prey can reproduce} \tag{2.13a}$$

$$Y + X \xrightarrow{k_2} 2\,Y \qquad\qquad \text{predator eats a prey and simultaneously reproduces} \tag{2.13b}$$

$$Y \xrightarrow{k_3} \varnothing \qquad\qquad\qquad\qquad\qquad \text{the predator dies} \tag{2.13c}$$

The first equation (2.13a) shows X produced by itself without interaction with anything. This desctiption is nothing like the classical binary chemical reaction, but can be used for more general settings: this can describe also an immigration (when something from outstide enters the system) or a reaction with a reactant in excess that can be considered as part of the environment, a condition for the reaction to occur but in such a large quantity that its density is unchanged by the reaction (in this case, $A + X \to 2\,X$, a prey eats A and then reproduces, but concentration of A is not affected by this). A similar analysis can be done for the term in equation (2.13c), where the predator dies, producing nothing but consuming the reactant; this description can also be

applied to emigration (when something exits the system). Another element to notice in equations (2.13a) and (2.13b) is the presence of X and Y respectively in both sides of the reaction: when computing the reaction rate it's easy to understand that only one respective unit is produced in both reactions.

To get the ODEs is sufficient to simply sum the effects of different reactions:

$$\begin{cases} \dot{x} = k_1\, x - k_2\, x\, y \\ \dot{y} = k_2\, x\, y - k_3\, y \end{cases} \tag{2.14}$$

These are known as the Lotka-Volterra equations for the predator and prey system.

Exercise 23: Lotka Volterra equations' stability and conservation law

Show that at stationarity the concentrations assume the values

$$\bar{x} = \frac{k_3}{k_2}, \qquad \bar{y} = \frac{k_1}{k_2}$$

but the Jacobian at $(\bar{x}, \bar{y})$ has pure imaginary eigenvalues
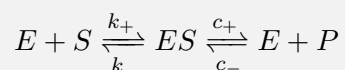
$$\lambda = \pm i \sqrt{k_1 k_3}$$

Show that the following is a non-linear conserved quantity (a *conservation law*)

$$V(x, y) = k_2(x + y) - k_3 \ln x - k_1 \ln y$$

2.2.4 Exercises over notable models

Exercise 24: Enzymatic reaction

Find the ODEs of the following enzymatic reaction:

$$E + S \underset{k_-}{\overset{k_+}{\rightleftharpoons}} ES \underset{c_-}{\overset{c_+}{\rightleftharpoons}} E + P$$

The reaction represents a typical interaction between a molecule S and an enzyme E in which a complex ES is formed. The complex, a union system between S and E decays in $E + P$ after some time, and in the end the all process can be seen as the enzyme E that transforms S into P in some specific time.

There are 4 dynamic variables whose reaction rates has to be described in this system, E, S, ES and P; even though it has been described for chemical purposes, this model has a wide variety of applications.

Exercise 25: Brusselator equations

Derive the ODEs for X and Y from the following reactions:

$$A \xrightarrow{k_1} X$$

$$B + X \xrightarrow{k_2} Y + D$$

$$2X + Y \xrightarrow{k_3} 3X$$

$$X \xrightarrow{k_4} E$$
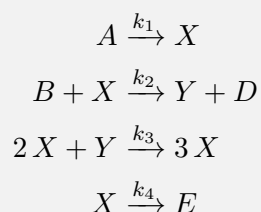
This is a theoretical model for an autocatalytic reaction (a reaction that allows one reactant to cause its own increase in concentration) for a non-equilibrium system proposed by Prigogine and studied up to today. It shows oscillatory behaviour, limit cycles and chaos

dynamic in differnt regions of the phase space.

Only X and Y have to be considered as dynamic variables, as it is assumed concentrations of A, B, D and E remain constant and are in excess (as a big reservoir).

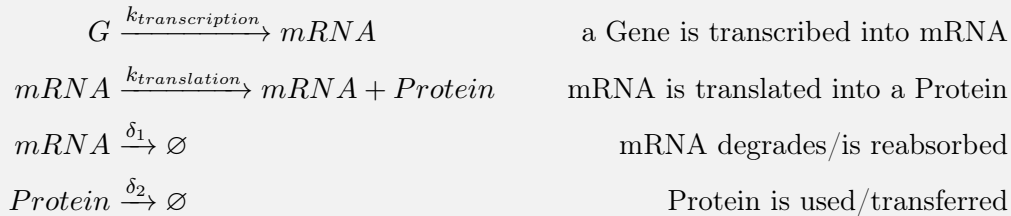**Exercise 26: Gene expression dynamics**

This model considers a simple model of gene expression where a gene is transcribed to mRNA, which is also translated into a protein:

$$G \xrightarrow{k_{transcription}} mRNA \qquad\qquad \text{a Gene is transcribed into mRNA}$$

$$mRNA \xrightarrow{k_{translation}} mRNA + Protein \qquad \text{mRNA is translated into a Protein}$$

$$mRNA \xrightarrow{\delta_1} \varnothing \qquad\qquad\qquad \text{mRNA degrades/is reabsorbed}$$

$$Protein \xrightarrow{\delta_2} \varnothing \qquad\qquad\qquad \text{Protein is used/transferred}$$

Derive the ODEs for $mRNA$ and $Protein$, the two dynamic variables in the previous eq.s. G is used as a representation of some subsrate that generates $mRNA$; obviously it is not so realistic, gene transcription requires more complex processes, but here it is assumed that the gene becomes ready after all of those.

It is important to notice that $mRNA$ does not degrade during translation, but after that both $mRNA$ and $Protein$ are consumed or removed from the system in some ways.
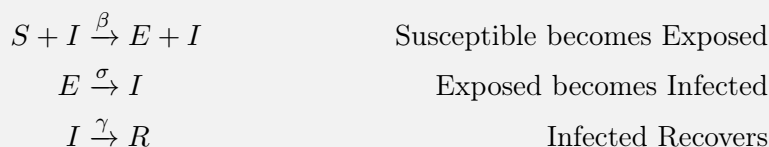
This is a rough model for gene expression, that is used for simple analysis and first approximation; even though this basic idea is still present in all its variations and more complex models (with activation process, more $mRNA$ types and sequences, ...).

The previous note is an important reminder of the modeling process, that can be expressed as:

1. start with a simple idea that describes the bases

2. try a stochastic implementation of the previous version

3. check if the stochastic analysis correctly predicts the intended bases:

   (a) if the previous model is enough to cover the bases, it is complete and can be variated at need in a second moment

   (b) if the model is not enough to cover the bases, it must be adjusted with some more complexity and then return to step 2.

Exercise 27: The SEIR model

Derive the ODEs for S, E, I and R from the following reactions:

$$S + I \xrightarrow{\beta} E + I \qquad\qquad \text{Susceptible becomes Exposed}$$

$$E \xrightarrow{\sigma} I \qquad\qquad\qquad \text{Exposed becomes Infected}$$

$$I \xrightarrow{\gamma} R \qquad\qquad\qquad \text{Infected Recovers}$$

This is a well known model in epidemiology, to study also population dynamics, chemistry, genome and biology, and can be seen as an evolution of the SIR model.

2.3 General chemical reactions

To make the law of mass action more universal, one may want to consider m <u>different chemical species</u> identified as x_i $i = 1, 2, ..., m$ which are involved in m <u>different reactions</u> of the form

$$\sum_{i=1}^{m} a_{\mathbf{i}j} X_i \underset{k_j^-}{\overset{k_j^+}{\rightleftharpoons}} \sum_{i=1}^{m} b_{i\mathbf{j}} X_i \qquad j = 1, 2, ..., n \tag{2.15}$$

<div align="center">different species   different reactions</div>
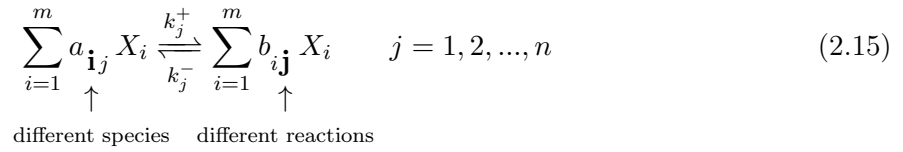
where a_{ij} and b_{ij} are stoichiometric coefficients that are all non-negative integers (can be zeros). Therefore it is possible to show that the ODEs are:

$$\dot{x}_i = \sum_{j=1}^{n} (b_{ij} - a_{ij}) \, r_j(\bar{x}) \qquad i = 1, 2, ..., m \tag{2.16}$$

where reaction rates are $\quad r_j(\bar{x}) \equiv k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}} - k_j^- \prod_{i=1}^{m} x_i^{b_{ij}} \quad$ for any $j = 1, 2, ..., n$

> **Exercise 28: Proof of general chemical equations ODEs**
>
> carefully prove the previous result: obtain (2.16) from (2.15)

The next question should be to find the conservation laws of eq. (2.16)
Let S be the $m \times n$ stoichiometric matrix defined as: $S_{ij} \equiv b_{ij} - a_{ij}$. The equations (2.16) can be written in vectorial form as:

$$\frac{\mathrm{d}}{\mathrm{d}t}\vec{x} = S\vec{r}(\bar{x}) \tag{2.17}$$

If it exits, a linear conservation law for the system (2.15) or (2.16) has the form

$$\frac{\mathrm{d}}{\mathrm{d}t} \sum_{i=1}^{m} c_i x_i = 0 \tag{2.18}$$

where c_i are (not all-zero) constants. If $\sum_i c_i x_i(t)$ is a constant of motion,

$$\sum_i c_i x_i(t) = \sum_i c_i x_i(0) = \vec{c}^\top \cdot \vec{x}(0)$$

where $\vec{c}^\top \equiv (c_1, c_2, ..., c_m)$. If equation (2.17) is multiplied by $\vec{c}^\top$, then

$$\vec{c}^\top \cdot \frac{\mathrm{d}}{\mathrm{d}t}\vec{x} = \vec{c}^\top \cdot S\vec{r} \overset{\underset{(2.17)}{\downarrow}}{=} \frac{\mathrm{d}}{\mathrm{d}t}\vec{c}^\top \cdot \vec{x}(0) \overset{\underset{(2.18)}{\downarrow}}{=} 0 \tag{2.19}$$

Equation (2.19) must hold true for all $\vec{r} \neq \vec{0}$, hence it must be

$$\vec{c}^\top S = 0 \qquad \text{or} \qquad S^\top \vec{c} = 0 \tag{2.20}$$

So, the conservation laws of the system of reactions in equation (2.15) are given by the non-zero elements $\vec{c} \in ker\left(S^\top\right)$, where $\vec{c}^\top \cdot \vec{x} = constant$. The number of linearly independent conservation laws is given by $dim\left[ker\left(S^\top\right)\right]$.

Example 9: General conservation laws

For the reaction

$$X + Y \to Z, \qquad S = \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}$$
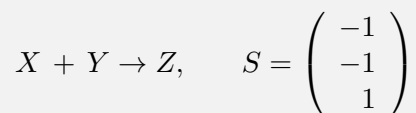
$$ker\left(S^{\top}\right) = \{(c_1, c_2, c_3) \,|\, c_1 + c_2 = c_3\}, \quad dim\left[ker\left(S^{\top}\right)\right] = 2$$

$$\vec{c}^{\top} \cdot \vec{x} = \sum_i c_i x_i = c_1 x + c_2 y + (c_1 + c_2)\, z = constant$$

Using the correct bases is possible to get:

$$(1, -1, 0) \longrightarrow x(t) - y(t) = constant$$
$$(1, 0, 1) \longrightarrow x(t) + z(t) = constant$$

2.4   Tools for the simulation of chemical reactions

Many tools and libraries are available for the numerical simulation of chemical reactions, here some links are provided:

- **COPASI** (free and professional tool) https://copasi.org/

- **LIBROADRUNNER** (library for C++/Python) https://www.libroadrunner.org/

- **List of other tools** https://sbml.org/software/#main-programming-libraries-and-tools

It is however a good practice to write down one's own code to check whether the basics of the theory have been understood.
The reaction shown until now should be implemented with stochastic algorithms, which account for the discrete nature of the particles. These tools will be provided in the next chapters.

Chapter 3

Turing Patterns

Fig. 3.1: Some examples of patterns that occur in nature.

This is the last deterministic model of this course. In the following section, we are going to describe, at its core, the simplest model of spatial pattern formation. By "pattern," we indicate a heterogeneous spatial structure. Examples include black and white stripes on a zebra, spots on the fur of a tiger, or stripes on a seashell (see Fig 3.1). The logician, computer scientist, code breaker Alan Turing (1912–1954) suggested a mathematical model to explain pattern emergence in his renowned article *The Chemical Basis of Morphogenesis* (1952). The framework for the model is deterministic reaction dynamics, where the species involved in the reactions are actual chemical species, such as skin pigments or their precursors.

These chemicals both react among themselves and diffuse inside the medium: the interplay between the two processes is what makes pattern emergence possible. Diffusion is usually regarded as a "homogenizing process," meaning that it tends to smooth out inhomogeneities inside a system (for instance, the diffusion of heat inside a medium makes its temperature homogeneous). The key rather counter-intuitive finding of Turing was that the process of diffusion, if coupled with reaction, can also have a destabilizing effect on the system, driving it out of its relatively homogeneous steady state. This mechanism is commonly referred to as a *diffusion-driven instability*.

Turing patterns are related to symmetry breaking in non-equilibrium systems and represent an example of emergent phenomena, namely, a phenomenon that emerges from the combination of processes, which on their own do not possess any property related to the phenomenon itself.

It's been some time since Turing's publication, and nowadays pattern formation has been studied extensively: many different models have been proposed, and their applications examined in a wide range of domains (e.g., network science). Obviously, we won't be able to cover everything the literature has to offer. The chapter is organized as follows:

- Section 1 introduces the modeling framework in the simplest case possible: one species only. We will see that with just one species, the process of diffusion effectively acts as a stabilizer for the spatially homogeneous solution.

- Section 2 deals with the two-species case. We will show that the diffusion process acts as a

stabilizer or a de-stabilizer depending on the ratio of the diffusivity constants, thus making room for the possibility of non-homogeneous solutions (patterns) to emerge.

- Section 3 highlights the key features and requirements that a reaction-diffusion model must have to allow for pattern formation. These requirements must be satisfied by every model, besides its level of complexity. We also discuss its specific details and motivations.

- Section 4 presents a practical example: the "activator-substrate depletion model" and illustrates the mathematical concepts developed with visuals obtained from numerical simulations.

For simplicity, we assume that the molecular species belong to a $1D$ finite domain $[0, L]$.

3.1 Reaction-diffusion with a single species

Let $[0, L]$ denote the finite domain that the species can occupy, and let $u(x,t)$ represent its concentration. A reaction-diffusion model in its general form is written as:

$$\frac{\partial u}{\partial t} = \overbrace{D\nabla^2 u}^{\text{diffusion}} + \overbrace{f(u)}^{\text{reaction}}, \tag{3.1}$$

where D is the diffusivity constant, and $f(u)$ represents the production rate of the molecule. Boundary conditions can vary without fundamentally affecting the results; for simplicity, we consider Dirichlet periodic boundary conditions:

$$u(x = 0, t) = u(x = L, t) \quad \forall \quad t > 0. \tag{3.2}$$

but the student is invited to work out the calculations with Neumann's zero flux boundary conditions too (see Exercise TODO). The reaction term $f(u)$ in Eq. (3.1) represents the production rate of the molecule u. It is typically chosen as a polynomial or rational function of u. For instance, one could assume the set of reactions:

$$\begin{cases} 3\,U \underset{k_-}{\overset{k_+}{\rightleftharpoons}} 2\,U \\ \varnothing \underset{\mu_-}{\overset{\mu_+}{\rightleftharpoons}} U \end{cases}$$
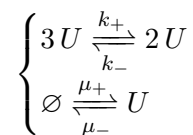
which give the reaction rate:

$$f(u) = \mu_+ + \mu_-\,u + k_-\,u^2 - k_+\,u^3.$$

of course, the choice of the reaction term is done with some biological motivation. For what concerns us, however, this aspects can be neglected. For now, we only care that f is continuous and derivable.

Spatially homogeneous solutions and their stability

If there exists a (spatially) uniform, stationary state $u(x,t) = u_0 > 0 \quad \forall\, (x,\,t)$, then it is also a root of the reaction term:

$$0 = \frac{\partial u}{\partial t} = f[u(x,t)] - D\frac{\partial^2 u(x,t)}{\partial x^2} = f[u_0]$$

Let us assume that such a state u_0 exists and that the first derivative of $f(u)$ is non-null, $f'(u_0) \neq 0$. This latter assumption is needed because we wish to address the *linear stability* of u_0. Say the system is in the steady uniform state and suppose that at $t = 0$ we introduce a
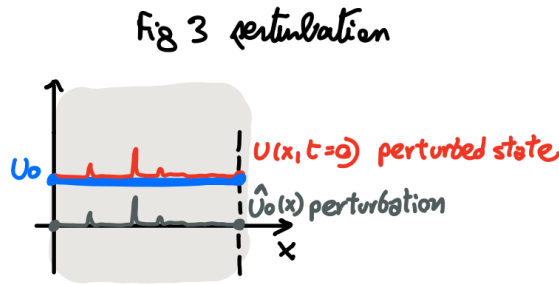
Fig. 3.2: Perturbation

small, inhomogeneous perturbation $\hat{u}(x,t)$ somewhere in the domain, so that we can rewrite the concentration $u(x,t)$ as:

$$u(x,t) = u_0 + \hat{u}(x,t) \quad \text{or} \quad \hat{u}(x,t) := u(x,t) - u_0 \qquad \text{with} \quad |\hat{u}(x,t)| \ll u_0.$$

How does the perturbation $\hat{u}(x,t)$ evolve in time? Plugging $\hat{u}$ into (Eq. 3.1):

$$\begin{cases} \frac{\partial}{\partial t}\, \hat{u}(x,t) & = f[u_0 + \hat{u}(x,t)] + D\frac{\partial^2}{\partial x^2}\, \hat{u}(x,t) \quad \forall x \in [0,L], \\[2mm] \hat{u}(0,t) & = \hat{u}(L,t) \qquad \text{(Dirichlet periodic BC)} \end{cases}$$

Since we are assuming that, initially, the perturbation is infinitesimally small, we can Taylor-expand the reaction term $f[u_0 + \hat{u}(x,t)]$ around u_0:

$$f[u_0 + \hat{u}(x,t)] \simeq f[u_0] + f'[u_0] \cdot \hat{u}(x,t)$$

and get the linearized equations:

$$\begin{cases} \frac{\partial \hat{u}(x,t)}{\partial t} & = f'[u_0] \cdot \hat{u}(x,t) + D\frac{\partial^2 \hat{u}(x,t)}{\partial x^2} \quad \forall x \in [0,L], \\[2mm] \hat{u}(0,t) & = \hat{u}(L,t) \quad \text{(Dirichlet periodic BC)} \end{cases} \qquad (3.3)$$

Stability conditions in absence of diffusion

If $D = 0$, then the general solution of Eq. (3.3) is simply:

$$\hat{u}(x,t) = \hat{u}_0(x) \cdot e^{f'(u_0)\,t} \quad \text{where} \quad \hat{u}_0(0) = \hat{u}_0(L) \qquad (3.4)$$

This implies that the perturbation dies out $(\lim_{t \to \infty} \hat{u}(x,t) = 0)$ for $f'(u_0) < 0$, whereas it explodes for $f'(u_0) > 0$. In the case $f'(u_0) = 0$, the linearized equations are not informative enough to deduce something, and we say that the equilibrium is *linearly neutrally stable*.

Stability conditions in presence of diffusion

When diffusion is present $(D > 0)$, then (Eq. 3.3) can be solved via separation of variables, i.e., using the ansatz:

$$u(x,t) = h(x) \cdot k(t).$$

Plugging this into equation (Eq. 3.3) we get

$$\begin{cases} h(x) \cdot \dot{k}(t) = D \cdot h''(x) \cdot k(t) + f'[u_0] \cdot h(x) \cdot k(t), \\ h(0) = h(L) = 0 \end{cases}$$

or equivalently:

$$\begin{cases} \frac{\dot{k}(t)}{k(t)} = D\frac{k''(x)}{k(x)} + f'[u_0] \\ h(0) = h(L) = 0 \end{cases}$$

On the left side, there is a function of t only, while on the right side there is a function of x only. There is no way that these can equal for all times and positions unless they are the same constant $\lambda \in \mathbb{R}$. Set this to be the case, then we have:

$$\begin{cases} \frac{h'(t)}{h(t)} = \lambda \\ D\frac{k''(x)}{k(x)} + f'[u_0] = \lambda \\ h(0) = h(L) = 0 \end{cases}$$

Which results in $h(t) = k_0 e^{\lambda t}$ for the temporal part. For the spatial part, rewrite:

$$\begin{cases} h''(x) + \left(\frac{f'[u_0]-\lambda}{D}\right) \cdot h(x) = 0 \\ h(0) = h(L) = 0 \end{cases}$$

So now there are several types of solutions:

case A: $\left(\frac{f'[u_0]-\lambda}{D}\right) > 0$

$$\begin{cases} h''(x) + \rho^2 h(x) = 0, \\ h(0) = h(L) = 0, \end{cases}$$

which gives:

$$\begin{cases} h(x) = A\cos(\rho x) + B\sin(\rho x) \\ h(0) = A = 0, \ h(L)^a = 0 \end{cases} \quad \Rightarrow \quad h_n(x) = B\sin\left(\frac{n\pi}{L}x\right), \quad n = 1, 2, \cdots$$

The relation of the constant λ_n to the wavenumber ρ_n is given by:

$$\lambda_n = \lambda(\rho_n^2) = f'[u_0] - D \cdot \left(\frac{n^2\pi^2}{L^2}\right) \tag{3.5}$$

___

[a]Here we explicitly assumed that the perturbation is null at the domain extrema. This simplifies the form of the solution, but the general case is almost identical. With $h(0) = h(L) = a > 0$, the solution would be $h(x) = \frac{a}{\cos\phi} \cdot \cos(\rho_n x + \phi)$ with $\rho_n = \frac{2\pi}{L} \cdot n$

case B: $\left(\frac{f'[u_0]-\lambda}{D}\right) = 0$:

$$\begin{cases} h''(x) = 0, \\ h(0) = h(L) = 0, \end{cases}$$

which has only the trivial solution:
$$h(x) \equiv 0.$$

case C: $\left(\frac{f'[u_0]-\lambda}{D}\right) < 0$:

$$\begin{cases} h''(x) - \rho^2 h(x) = 0, \\ h(0) = h(L) = 0, \end{cases}$$

which gives:

$$h(x) = A\cosh(\rho x) + B\sinh(\rho x) \quad \Rightarrow \quad \begin{cases} h(0) = A = 0, \\ h(L) = 0, \end{cases}$$

which, again, has only the trivial solution:

$$h(x) \equiv 0.$$

Indeed, since (Eq. 3.3) is linear, any linear combination of the solutions found is again a solution. Therefore, the most general solution of the type $u(x,t) = h(x) \cdot k(t)$ that solves the (Eq. 3.3) *together with* the boundary conditions we imposed is given by the Fourier series:

$$\hat{u}(x,t) = \sum_{n=1}^{+\infty} \alpha_n \sin(\rho_n x) \cdot e^{\lambda(\rho_n^2)t} \tag{3.6}$$

where the $\{\alpha_n\}_{n=1}^{+\infty}$ are determined from the initial perturbation $\hat{u}_0(x)$. From now on, though we have not proven it, we regard (Eq. 3.6) as the most general solution of (Eq. 3.3) [1]. Now let us come back to our original question: is the steady state stable in presence of diffusion ($D > 0$)? This depends on the sign of the $\{\lambda_n\}$ that appear in the Fourier series. The n-th mode will be stable when $\mathcal{R}e\{\lambda_n\} < 0$. The steady state is linearly stable if all the modes are stable. Notice from (Eq. 3.5) that it is sufficient that $\lambda_1 < 0$, and this happens if:

$$D > f'[u_0] \cdot \left(\frac{L}{\pi}\right)^2.$$

This last equation implies that, unlike in the previous case ($D = 0$), even if $f'[u_0] > 0$, the homogeneous steady state can still be stable, provided that the diffusion constant is sufficiently high. In this sense, we state that *diffusion has a stabilizing effect on a 1 species system*. We will soon see that this is no longer (always) true when a second species is added.

Comment: Of course, we can also look at (Eq. 3.5) the other way around: if D is fixed and $f'[u_0] > 0$, the stability depends on the size L of the domain. Stability occurs if $L < L_c(D)$, outside this threshold, instability arises, where:

$$L_c(D) = \pi\sqrt{\frac{D}{f'[u_0]}}.$$

Exercise 29: Neumann zero flux boundary conditions

Repeat the calculations that lead to (Eq: 3.5), but assuming Neumann zero-flux boundary conditions instead, i.e.

$$\begin{cases} \partial_t u(x = 0, t) = 0 \\ \partial_t u(x = L, t) = 0 \end{cases} \quad \forall\, t > 0$$

Does (Eq: 3.5) change?

3.2 Two-species system

For a system of two (or more) interacting species, diffusion can also have a *destabilizing* effect on homogeneous solutions. This opens the possibility for pattern emergence.

---

[1] Is it, really?

Let $u(x,t)$ and $v(x,t)$ be the concentrations of the species living in the 1D domain $x \in [0, L]$, which satisfy the following reaction-diffusion equations:

$$
\begin{cases}
\dot{u} = f(u,\, v) + D_u \frac{\partial^2}{\partial x^2}\, u \\[2mm]
\dot{v} = g(u,\, v) + D_v \frac{\partial^2}{\partial x^2}\, v \\[2mm]
\frac{\partial u}{\partial x}(x=0, t) = \frac{\partial u}{\partial x}(x=L, t) = 0 \\[2mm]
\frac{\partial v}{\partial x}(x=0, t) = \frac{\partial v}{\partial x}(x=L, t) = 0
\end{cases}
\tag{3.7}
$$

where we imposed Neumann zero-flux boundary conditions. Here, f and g are smooth functions, and $D_u, D_v > 0$ are the diffusivity constants of u and v, respectively. As before, let us assume that there exists a stationary state (u_0, v_0),

$$
\begin{cases}
f(u_0, v_0) &= 0, \\
g(u_0, v_0) &= 0,
\end{cases}
$$

and let us study its linear stability with and without diffusion.

As in the previous section, we introduce a small, non-homogeneous perturbation $(\hat{u}_0, \hat{v}_0)$ in the domain and look at the time evolution of the perturbation

$$
\begin{cases}
\hat{u}(x,t) &= u(x,t) - u_0, \\
\hat{v}(x,t) &= v(x,t) - v_0.
\end{cases}
$$

By Taylor expansion of (Eq. 3.7), we get:

$$
\begin{cases}
\frac{\partial}{\partial t} \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix} = \begin{pmatrix} f_u & f_v \\ g_u & g_v \end{pmatrix} \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix} + \begin{pmatrix} D_u \frac{\partial^2}{\partial x^2} & 0 \\ 0 & D_v \frac{\partial^2}{\partial x^2} \end{pmatrix} \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix}, \\[4mm]
\frac{\partial}{\partial x} \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix}(x=0, t) = \frac{\partial}{\partial x} \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix}(x=L, t) = \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\end{cases}
\tag{3.8}
$$

where $\{f_u, f_v, g_u, g_v\}$ indicate the derivatives calculated at the steady state, e.g.

$$
f_u = \frac{\partial f}{\partial u}(u_0, v_0)
$$

For simplicity of notation, let us rename $\hat{u} := \begin{pmatrix} \hat{u} \\ \hat{v} \end{pmatrix}$, the concentration vector. Then more compactly, we can write the above as:

$$
\begin{cases}
\frac{\partial}{\partial t}\, \hat{u}(x,t) = \left[J + D \frac{\partial^2}{\partial x^2} \right] \hat{u}(x,t), \\[2mm]
\frac{\partial}{\partial x}\, \hat{u}(x=0, t) = \frac{\partial \hat{u}}{\partial x}(x=L, t) = 0,
\end{cases}
\tag{3.9}
$$

We now aim to find the general solution of (Eq. 9). With the previous section in mind, we use the ansatz:

$$
\hat{u}_k(x,t) = \vec{a}_k \cdot e^{ikx + \lambda(k^2)t}
\tag{3.10}
$$

Comment: this is a complex-valued function, but it its real and imaginary part are also valid solutions, and their are physically meaningful. In fact, if $\hat{u}$ solves the differential equation, its complex conjugate $\overline{\hat{u}}$ also solves the same equation. The real part is rewritten as $\mathbb{Re}[\hat{u}] = \frac{\hat{u} + \overline{\hat{u}}}{2}$. Since equation 3.9 is linear, $\mathbb{Re}[\hat{u}]$ is a solution.

Substituting (Eq. 3.10) into (Eq. 3.9) leads to a k-dependent eigenvalue problem:

3.3   Important remarks

3.4   The Activator - Substrate Deplection model

The Activator - Substrate Deplection model is a simple model to describe the interaction between two species, the Activator U and the Substrate V, when the activator is autocatalyic[2] and consumes the substrate, while degrading. There is also a continuous and constant production of the substrate.

$$2\,U + V \xrightarrow{\bar{\mu}} 3\,U \qquad \text{autocatalyic production of activator U consuming substrate V}$$

$$U \xrightarrow{\gamma} \varnothing \qquad\qquad\qquad\qquad\qquad\qquad \text{decay of the activator U}$$

$$\varnothing \xrightarrow{\beta} V \qquad\qquad\qquad\qquad\qquad \text{continuous production of the substrate V}$$
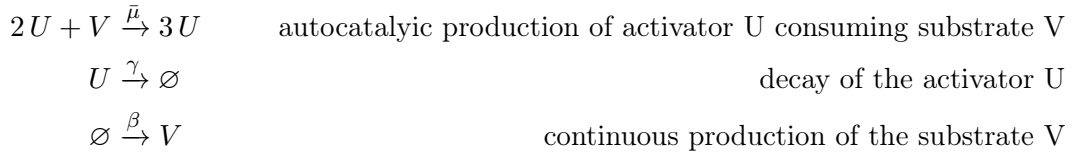
To see if Turing patterns can occur, the conditions explained in section 3.3 must be met. The ODEs for the reactions rates of the reactions without diffusivity effects are:

$$\begin{cases} \dot{u} = \bar{\mu}\,u^2\,v - \gamma\,u & = f(u,v) \\ \dot{v} = \beta - \bar{\mu}\,u^2\,v & = g(u,v) \end{cases}$$

The reaction-diffusion equation obtained adding spacial diffusion interaction is

$$\begin{cases} \dot{u} = D_1\,\nabla^2 u + \bar{\mu}\,u^2\,v - \gamma\,u \\ \dot{v} = D_2\,\nabla^2 v - \bar{\mu}\,u^2\,v + \beta \end{cases} \tag{3.11}$$

To find some Turing patterns is necessary to determin the correct region of parameters where to search: the conditions to be met for Turing Patterns to appear depend on parameters, and for this system these are 5 free parameters $(\bar{\mu}, \gamma, \beta, D_1, D_2)$. Up to this point the parameter space is 5 dimensional, the system has to be simplyfied before being studied.
This is a good practice: before start studying the system it is important to make the variables **dimensionless** and reduce to the **minimum** the **number of free parameters**.

3.4.1   Rescaling parameters - a general procedure

[3] Typically reactions does not depend on the singles parameters but rather on a certain combination of their ratios: finding a way to obtain indipendent equations to control the parameters can simplify a lot the analysis. This procedure is called **Nondimensionalization** and can be used to reduce the number of indipendent parameters while still being able to explore the full range of behaviour of an equation dynamics.
The core and simple idea behind this operation is the homogeneity of the terms composing the equation: each variable has its own dimension (length, time, density) but in order to be summed to the other terms has to be rescaled by appropriate parameters. Starting from this fundamental assumption, the equation is rewritten and variables rescaled in order to make every term dimensionless (its dimension becomes the unit). This leads to some benefits:

1. reduced number of parameters, only their dimensionless combinations can appear

2. relative magnitudes of different terms are easier to compare

3. ratios and quantities that controls the dynamics became intuitive

To help this procedure the *Buckingham π Theorem* proves useful: it states that

---

[2]For a quick reminder, a reaction is catalytic if a species increases the production rate of another one, typically not being consumed during the process; it's said autocatalyic if a species itself is involved in its own production and its concentration increases its own production rate.

[3][EN] this section was added to provide a more general context for the subsequent counts

> *A system described by n variables and parameters, built from r independent dimensions, is completely described by $p = n - r$ dimensionless groups.*

This very powerful result does not provide an unique way to determin those groups. In the context of reaction dynamics it has been found the following procedure to be generally effective. Calling x_i all the variables in the equations (not the parameters):

1. For each variable, time included, is defined a dimensionless version such that $x_i = x_{i,d}\tilde{x}_i$: $\tilde{x}_i$ is called the dimensionless variable and the constant $x_{i,d}$ imparts the dimension of x_i.

2. These expressions are substituted into the dynamic equations

3. The equation must be rearranged such that every term is now dimensionless. The result will display dimensionless ratios and products of the $x_{i,d}$ and original system parameters.

4. Those dimensionless ratios (or products) can be defined as dimensionless parameters.

5. Choosing expressions for $x_{i,d}$ that minimize the number of dimensionless parameters should give the result predict by *Buckingham π Theorem*: the sum between the number of dimensionless variables and parameters should be p.

3.4.2   Rescaling parameters

The dimensional analysis of the previous system is , with some abuse of notation

$$\begin{cases} [\dot{u}] = \frac{N}{L^2 T} = [D_1] \left[\nabla^2 u\right] + [\bar{\mu}] \left[u^2\right] [v] - [\gamma] [u] = \frac{L^2}{T}\frac{N}{L^4} + \frac{L^4}{T N^2}\left(\frac{N}{L^2}\right)^2\frac{N}{L^2} - \frac{1}{T}\frac{N}{L^2} \\ [\dot{v}] = \frac{N}{L^2 T} = [D_2] \left[\nabla^2 v\right] - [\bar{\mu}] \left[u^2\right] [v] + [\beta] = \frac{L^2}{T}\frac{N}{L^4} - \frac{L^4}{T N^2}\left(\frac{N}{L^2}\right)^2\frac{N}{L^2} + \frac{N}{L^2 T} \end{cases}$$

where here $[...]$ indicates the dimension of the argument, L is length, T time, N unit counter of the two species.

There are three independent dimensions (L, T, N) and nine between variables and parameters $(u, v, x, t, \bar{\mu}, \gamma, \beta, D_1, D_2)$ so for the *Buckingham π Theorem* should be possible to write the problem using six independent dimensionless groups (4 variables and 2 parameters). Following the procedure, every variable is written as its dimensionless version multipled by its dimension:

$$\begin{cases} \frac{u_d}{t_d}\frac{\mathrm{d}\tilde{u}}{\mathrm{d}\tilde{t}} = D_1 \frac{u_d}{x_d^2}\frac{\partial^2\tilde{u}}{\partial\tilde{x}^2} + \bar{\mu}\, u_d^2\tilde{u}^2\, v_d\, \tilde{v} - \gamma\, u_d\, \tilde{u} \\ \frac{v_d}{t_d}\frac{\mathrm{d}\tilde{v}}{\mathrm{d}\tilde{t}} = D_2 \frac{v_d}{x_d^2}\frac{\partial^2\tilde{v}}{\partial\tilde{x}^2} - \bar{\mu}\, u_d^2\tilde{u}^2\, v_d\, \tilde{v} + \beta \end{cases}$$

dividing now first equation by $\frac{u_d}{t_d}$ and the second one by $\frac{v_d}{t_d}$ the problem is reduced to

$$\begin{cases} \frac{\mathrm{d}\tilde{u}}{\mathrm{d}\tilde{t}} = D_1 \frac{t_d}{x_d^2}\frac{\partial^2\tilde{u}}{\partial\tilde{x}^2} + \bar{\mu}\, u_d\, v_d\, t_d\, \tilde{u}^2\, \tilde{v} - \gamma\, t_d\, \tilde{u} \\ \frac{\mathrm{d}\tilde{v}}{\mathrm{d}\tilde{t}} = D_2 \frac{t_d}{x_d^2}\frac{\partial^2\tilde{v}}{\partial\tilde{x}^2} - \bar{\mu}\, u_d^2\, t_d\, \tilde{u}^2\, \tilde{v}v + \frac{t_d}{v_d}\beta \end{cases}$$

Now the values for the dimensions must be defined to make equations dimensionless. A obvious choice for t_d could be $t_d = \gamma^{-1}$; is defined $x_d = \sqrt{\frac{D_1}{\gamma}}$ such as the constant $d = \frac{D_2}{D_1}$ can appear; finally the dimensions for u and v are defined to make the resulting equation dimensionless.

This is equivalent to rescale with a change of variables such as:

$$\text{scaling time: } t' = \gamma\, t \qquad \text{scaling space: } (x', y') = \sqrt{\frac{\gamma}{D_1}}(x, y)$$

$$\begin{cases} \frac{dt'}{dt}\frac{du}{dt'} = D_1 \left(\frac{\partial x'}{\partial x}\right)^2 \frac{\partial^2 u}{\partial x'^2} + \bar{\mu}\, u^2\, v - \gamma\, u \\ \frac{dt'}{dt}\frac{dv}{dt'} = D_2 \left(\frac{\partial x'}{\partial x}\right)^2 \frac{\partial^2 v}{\partial x'^2} - \bar{\mu}\, u^2\, v + \beta \end{cases}$$

$$\begin{cases} \gamma\, \dot{u} = D_1 \frac{\gamma}{D_1} \nabla^2 u + \bar{\mu}\, u^2\, v - \gamma\, u \\ \gamma\, \dot{v} = D_2 \frac{\gamma}{D_1} \nabla^2 v - \bar{\mu}\, u^2\, v + \beta \end{cases}$$

$$\begin{cases} \dot{u} = \nabla^2 u + \frac{\bar{\mu}}{\gamma}\, u^2\, v - u \\ \dot{v} = d\, \nabla^2 v - \frac{\bar{\mu}}{\gamma}\, u^2\, v + \frac{\beta}{\gamma} \end{cases} \qquad \text{for } d = \frac{D_2}{D_1} \tag{3.12}$$

now focusing on making all terms dimensionless it is possible to notice some combinations. Now in the dimensionless form the homogeneity condition can be applied to the parameters and the dimensions so

$$\text{for} \qquad \begin{cases} \frac{d\tilde{u}}{d\tilde{t}} = \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} + \frac{\bar{\mu}\, u_d\, v_d}{\gamma}\, \tilde{u}^2\, \tilde{v} - \tilde{u} \\ \frac{d\tilde{v}}{d\tilde{t}} = d\, \frac{\partial^2 \tilde{v}}{\partial \tilde{x}^2} - \frac{\bar{\mu}\, u_d^2}{\gamma}\, \tilde{u}^2\, \tilde{v} + \frac{\beta}{\gamma\, v_d} \end{cases}$$

$$\frac{\bar{\mu}\, u_d\, v_d}{\gamma} = 1 \qquad \frac{\beta}{\gamma\, v_d} = \frac{\bar{\mu}\, u_d^2}{\gamma}$$

$$\text{that gives} \qquad u_d = \frac{\beta}{\gamma} \qquad v_d = \frac{\gamma^2}{\beta\, \bar{\mu}}$$

that is equivalent to rescale the densities as follows:

$$\text{scaling activator: } u' = \frac{\gamma}{\beta} u \qquad \begin{cases} \frac{\partial u}{\partial u'}\dot{u}' = \frac{\partial u}{\partial u'}\nabla^2 u' + \left(\frac{\partial u}{\partial u'}\right)^2 \frac{\bar{\mu}}{\gamma}\, u'^2\, v - \frac{\partial u}{\partial u'} u' \\ \dot{v} = d\, \nabla^2 v - \left(\frac{\partial u}{\partial u'}\right)^2 \frac{\bar{\mu}}{\gamma}\, u'^2\, v + \frac{\beta}{\gamma} \end{cases}$$

$$\begin{cases} \dot{u}' = \nabla^2 u' + \frac{\beta}{\gamma}\frac{\bar{\mu}}{\gamma}\, u'^2\, v - u' \\ \dot{v} = d\, \nabla^2 v - \left(\frac{\beta}{\gamma}\right)^2 \frac{\bar{\mu}}{\gamma}\, u'^2\, v + \frac{\beta}{\gamma} \end{cases}$$

$$\text{scaling substrate: } v' = \frac{\bar{\mu}\, \beta}{\gamma^2} v \qquad \begin{cases} \dot{u}' = \nabla^2 u' + \frac{\partial v}{\partial v'}\frac{\beta, \bar{\mu}}{\gamma^2}\, u'^2\, v' - u' \\ \frac{\partial v}{\partial v'}\dot{v}' = d\, \frac{\partial v}{\partial v'}\nabla^2 v' - \frac{\partial v}{\partial v'}\frac{\bar{\mu}\beta^2}{\gamma^3}\, u'^2\, v' + \frac{\beta}{\gamma} \end{cases}$$

$$\begin{cases} \dot{u}' = \nabla^2 u' + \frac{\gamma^2}{\bar{\mu}\, \beta}\frac{\beta\, \bar{\mu}}{\gamma^2}\, u'^2\, v' - u' \\ \dot{v}' = d\, \nabla^2 v' - \frac{\bar{\mu}\beta^2}{\gamma^3}\, u'^2\, v' + \frac{\beta}{\gamma}\frac{\beta\, \bar{\mu}}{\gamma^2} \end{cases}$$

$$\begin{cases} \dot{u}' = \nabla^2 u' + u'^2\, v' - u' \\ \dot{v}' = d\, \nabla^2 v' - \frac{\bar{\mu}\beta^2}{\gamma^3}\, u'^2\, v' + \frac{\bar{\mu}\beta^2}{\gamma^3} \end{cases}$$

where is now possible to define the new parameter μ such that the equations can be expressed using only two parameters. Changing the name of the dynamic variables to be u, v again:

$$\begin{cases} \dot{u} = \nabla^2 u + u^2\, v - u \\ \dot{v} = d\, \nabla^2 v + \mu\left(1 - u^2\, v\right) \end{cases} \qquad \text{for } \mu = \frac{\bar{\mu}\, \beta^2}{\gamma^3} \tag{3.13}$$

This system is now, as anticipated, fully described by only two independent parameters, and its behaviour can be represented in a two dimensional space.

3.4.3 Parametric analysis

Once the equations have been reduced to the minimum parameters' size, it's much easier to analyze the behaviours that leads to the Turing patterns formation. As seen in the previous

sections, in order to a pattern to be able to appear, the system must be linearly stable around its steady state for the spacial homogeneous part of the equation. This can be obtained imposing:

$$
\begin{cases} \dot{u}\big|_{u_0,v_0} = u_0^2\, v_0 - u_0 = 0 \\ \dot{v}\big|_{u_0,v_0} = \mu\left(1 - u_0^2\, v_0\right) = 0 \end{cases}
\quad\Rightarrow\quad
\begin{cases} u\left(u_0\, v_0 - 1\right) = 0 \\ \left(1 - u_0^2\, v_0\right) = 0 \end{cases}
$$

Neglecting the trivial solution $u_0 = 0$

$$
\begin{cases} u_0\, v_0 = 1 \\ 1 - u_0 \cdot 1 = 0 \end{cases}
\qquad
\begin{cases} u_0 = 1 \\ v_0 = 1 \end{cases}
$$

obtaining the steady state (u_0, v_0). Now it is possible to linearize the system in the neighbourhood of this point, calculating the Jacobian for the as usual defined functions $f(u,v), g(u,v)$

$$
\begin{cases} \dot{u} = f(u,v) \\ \dot{v} = g(u,v) \end{cases}
\quad\Rightarrow\quad
J_0(u,v) = \begin{pmatrix} \partial_u f(u,v) & \partial_v f(u,v) \\ \partial_u g(u,v) & \partial_v g(u,v) \end{pmatrix}
$$

$$
J_0(u_0,v_0) = \begin{pmatrix} 2\,u\,v - 1 & u^2 \\ -2\,\mu\,u\,v & -\mu\,u^2 \end{pmatrix}\Bigg|_{u_0,v_0} = \begin{pmatrix} 1 & 1 \\ -2\mu & -\mu \end{pmatrix}
$$

imposing now that the system is stable without diffusion corrisponds to requiring negative eigenvalues for J_0, so

$$
\mathrm{Tr}\left(J_0\right)\Big|_{u_0,v_0} = 1 - \mu < 0 \quad\Rightarrow\quad \mu > 1
$$

$$
\det\left(J_0\right)\Big|_{u_0,v_0} = -\mu + 2\,\mu > 0 \quad\Rightarrow\quad \mu > 0
$$

satisfied those the linearized system is stable around the steady state, and such is for $\mu > 1$. The second requirement for Turing Patterns to appear is the diffusion-driven instability, such as the condition of instability for the linearized system in presence of diffusion. To verify this, the matrix J can be analyzed

$$
J = J_0 - k^2 D = \begin{pmatrix} 2\,u\,v - 1 & u^2 \\ -2\,\mu\,u\,v & -\mu\,u^2 \end{pmatrix} - k^2 \cdot \begin{pmatrix} 1 & 0 \\ 0 & d \end{pmatrix}
$$

$$
J(u_0,v_0) = \begin{pmatrix} 2\,u\,v - 1 - k^2 & u^2 \\ -2\,\mu\,u\,v & -\mu\,u^2 - k^2 d \end{pmatrix}\Bigg|_{u_0,v_0} = \begin{pmatrix} 1 - k^2 & 1 \\ -2\mu & -\mu - k^2 d \end{pmatrix}
$$

As seen before, for the patterns to be possible the matrix J have to admit at least one positive real-part eigenvalue. Following the derivation used in section 3.2, it is possibile to determin different areas of behaviour through eigenvalues classification.
The easiest passage is to analyze its invariants:

$$
\mathrm{Tr}\left(J\right) = 1 - \mu - k^2(1 + d) < 0 \quad \text{as seen for conditions on } J_0
$$

$$
\det\left(J\right) = \left(1 - k^2\right)\left(-\mu - k^2 d\right) + 2\mu \overset{?}{<} 0 \quad \text{requirement to have at least one } \mathrm{Re}\{\lambda\} > 0
$$

$$
\underbrace{d\,k^4}_{d\,k^4 > 0} - k^2\left(d - \mu\right) + \underbrace{\mu}_{\mu > 0} < 0 \quad\Rightarrow\quad k^2\left(d - \mu\right) > 0 \Rightarrow \mu < d
$$

This is, as already seen, a necessary but not sufficient requirement. To get a stroger result one must require that the minimum value of $\det(J)$ is negative, and so there exists a range of values

for k^2 in which Turing Patterns may occur.

$$\frac{\partial \det\left(J(k^2)\right)}{\partial(k^2)}\bigg|_{k_{min}^2} = 0$$

$$0 = 2\,d\,k_{min}^2 - d + \mu \qquad k_{min}^2 = \frac{d-\mu}{2\,d}$$

$$\det(J)\bigg|_{k_{min}^2} = \frac{(d-\mu)^2}{4\,d} - \frac{(d-\mu)^2}{2\,d} + \mu = \mu - \frac{(d-\mu)^2}{4\,d}$$

$$\det(J)\bigg|_{k_{min}^2} \stackrel{?}{<} 0 \qquad \frac{4\,d\,\mu - d^2 - \mu^2 + 2\,d\,\mu}{4\,d} < 0$$

$$0 < \mu^2 + d^2 - 6\,d\,\mu \quad \implies \quad 1 < \mu < d\left(3 - 2\sqrt{2}\right)$$

obtaining the condition that represents the critical diffusivity line for $\mu(d)$. The stability conditions for the homogeneous system impose $\mu \geq 1$ so the minimal critical diffusivity corresponds to $1 = \mu = (3 - 2\sqrt{2})d_c \Rightarrow d_c = 3 + 2\sqrt{2}$.

It is possible to analyze the whole spectrum of values the parameters can assume and costruct a linear stability diagram, a map of the $d - \mu$ plane identifying which region of parameter space have linear stability properties.

Starting from the analysis of the eigenvalues for J_0 three macro areas emerge:

$$\det\left(J_0 - \lambda\mathbb{1}\right) = \lambda^2 - \lambda\,\mathrm{Tr}(J_0) + \det(J_0)$$

$$\lambda_{1,2} = \frac{\mathrm{Tr}(J_0) \pm \sqrt{\mathrm{Tr}(J_0)^2 - 4\,\det(J_0)}}{2}$$

$$Tr(J_0)^2 - 4\,\det(J_0) = (1 - \mu)^2 - 4\,(\mu)$$

$$= 1 + \mu^2 - 2\,\mu - 4\,\mu = \mu^2 - 6\,\mu + 1$$

$$Tr(J_0)^2 - 4\,\det(J_0) \geq 0 \Leftrightarrow \mu^2 - 6\,\mu + 1 \geq 0$$

$$\Leftrightarrow 0 < \mu < 3 - 2\sqrt{2} \vee \mu > 3 + 2\sqrt{2}$$

combining this with the previous result for J_0 the relevant regions are:

1. $\mu > 1$:
   where λ_0 eigenvalues of J_0 have negative value real part (linear stability)

2. $3 - 2\sqrt{2} < \mu < 1$:
   where λ_0 have positive-value real part and non-zero imaginary part (oscillatory behaviour)

3. $0 < \mu < 3 - 2\sqrt{2}$:
   where λ_0 have positive-value real part and zero imaginary part (linear instability)

For each of these the behaviour of λ eigenvalues of J must be studied. As seen, in the region (1) there is at least one positive-valued λ if $\mu < d\left(3 - 2\sqrt{2}\right)$, enabling Turing patterns to form in that region, otherwise the system remains stable.

For the other two areas the complete analysis of λ should be performed, to compare their values with those of λ_0.

$$\det\left(J - \lambda\mathbf{1}\right) = \lambda^2 - \lambda\,\mathrm{Tr}(J) + \det(J)$$

$$\lambda_{1,2} = \frac{\mathrm{Tr}(J) \pm \sqrt{\mathrm{Tr}(J)^2 - 4\,\det(J)}}{2}$$

$$Tr(J)^2 - 4\,\det(J) = \left(1 - \mu - k^2(1+d)\right)^2 - 4\left(d\,k^4 - k^2\,(d-\mu) + \mu\right)$$

$$= k^4\,(1-d)^2 - 2\,k^2\,(1-d)\,(1+2\,\mu) + \left(\mu^2 - 6\,\mu + 1\right)$$

once the values for λ have been found, they should be compared with λ_0, to see where the maximum value for the real part occurs. If the system present a more instable behaviour in presence of diffusion (a grater Re$\{\lambda\}$ than all Re$\{\lambda_0\}$), Turing pattern may occur. It is often easier to take a "brute force" approach and compute the eigenvalues for each pair of parameters values for a range of k values, and then display the result as a color coded image, as it has been done in image 3.3. The gray scale and the number of the areas has been assigned according to the different class of eigenvalues that have been obtained, as in the following tables:

Region	Eigenvalues
1	$\forall\lambda_0 \ \mathrm{Re}\{(\lambda_0)\} < 0, \ \forall\lambda, \ \mathrm{Re}\{(\lambda)\} < 0$
2	$\forall\lambda_0 \ \mathrm{Re}\{(\lambda_0)\} < 0, \ \exists\lambda, |\ \mathrm{Re}\{(\lambda)\} > 0$
3	$\forall\lambda_0 \ \mathrm{Re}\{(\lambda_0)\} > 0, \ \mathrm{Im}\{(\lambda)\} \neq 0, \ \forall\lambda, \ \mathrm{Re}\{(\lambda)\} < \mathrm{Re}\{(\lambda_0)\}$
4	$\forall\lambda_0 \ \mathrm{Re}\{(\lambda_0)\} > 0, \ \mathrm{Im}\{(\lambda)\} \neq 0, \ \exists\lambda, |\ \mathrm{Re}\{(\lambda)\} > \mathrm{Re}\{(\lambda_0)\}\forall\lambda_0; \ \mathrm{Im}\{(\lambda)\} = 0$
5	$\forall\lambda_0 \ \mathrm{Re}\{(\lambda_0)\} > 0, \ \mathrm{Im}\{(\lambda)\} = 0, \ \forall\lambda, \ \mathrm{Re}\{(\lambda)\} < \mathrm{Re}\{(\lambda_0)\}$
6	$\forall\lambda_0 \ \mathrm{Re}\{(\lambda_0)\} > 0, \ \mathrm{Im}\{(\lambda)\} = 0, \ \exists\lambda, |\ \mathrm{Re}\{(\lambda)\} > \mathrm{Re}\{(\lambda_0)\}\forall\lambda_0$

Region	Description
1	Homogeneous steady state stable
2, 6	Turing patterns formation (where inibitor diffuses faster than activator)
3	Oscillating homogeneous patterns
4	Possible Turing patterns, depending on initial conditions (oscillatory instability)
5	Homogeneous unbounded growth

Fixing a certain value for d it is possible to discuss the response of the system for small changes of μ. Taking for example a value $d = 9$ as in figure 3.3, the line crosses 5 different regions: starting at a value $\mu = 1$ and increasing by little variation ϵ, at $\mu + \epsilon$ a first pattern starts to emerge, in the beginning for only a single wavenumber k, then increasing ϵ more wavenumber became available, and multiple patterns arise, until for $\epsilon >> 0$ the critical line is crossed and the higher reaction rate of the substrate makes pattern impossible to observe, and the homogeneous range starts again.

It is important to underline that the eigenvalues λ_0 corresponds to the wavenumber $k = 0$, by the definition of J, and the value of the real part of each λ rapresents the weight given to each wavenumber in the spectral linear decomposition of the system: if the most significant term corresponds to λ_0 the system is homogeneous as the main behaviour presents no oscillation.
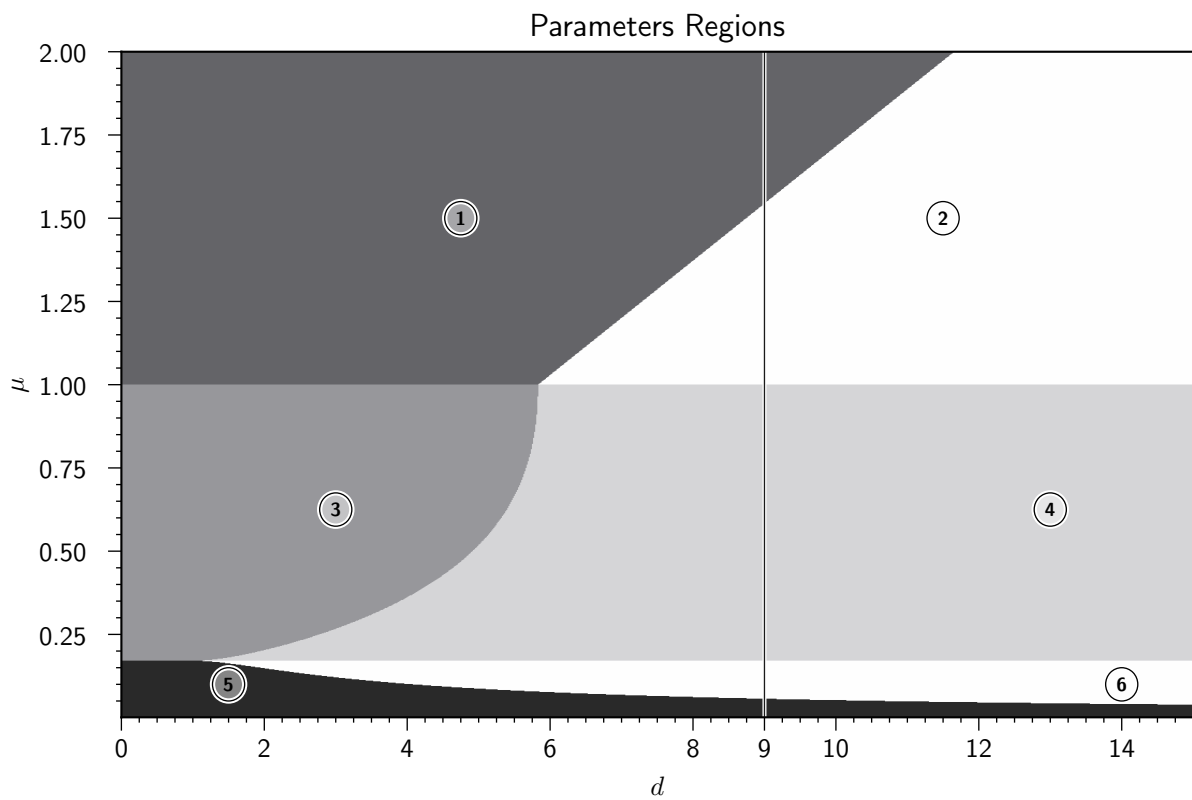
Fig. 3.3: Regions of possible patterns formation for different values of parameters.

Chapter 4

Solutions to the exercises

4.1 Chapter 1: Mathematical Tools

Exercise 1: C.F. of a uniform distribution

Given a random variable x drawn from a uniform distribution $U([a,b])$, calculate the c.f. of $p(x)$ where

$$p(x) = \begin{cases} 1 & \frac{1}{b-a} \in [a,b] \\ 0 & \text{elsewhere} \end{cases}$$

Sol.

$$\varphi(k) = \int_{\mathbb{R}} e^{ikx}\, p(x)\, \mathrm{d}x = \int_a^b e^{ikx}\, \frac{1}{b-a}\, \mathrm{d}x = \frac{1}{b-a}\left[\frac{1}{ik}e^{ikx}\right]_a^b = \frac{-i}{k(b-a)}e^{ik(b-a)}$$

Exercise 2: C.F of a γ-distribution

Given a random variable x drawn from a γ-distribution $\gamma(\alpha, \beta)$, with $\alpha > 0$, $\beta > 0$ prove that such distribution is normalized and calculate the c.f. of $q(x)$ where

$$q(x) = \gamma(\alpha, \beta) = \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1}\, e^{-\beta x} \qquad (0 \leq x \leq \infty \text{ or } x \in \mathbb{R}^+)$$

where $\Gamma(\alpha)$ represent the gamma function defined as usual:

$$\Gamma(z) = \int_0^\infty t^{z-1}\, e^{-t}\, \mathrm{d}t$$

Sol. To prove normalization:

$$\int_{\mathbb{R}^+} q(x)\, \mathrm{d}x = \int_0^\infty \frac{\beta^\alpha}{\Gamma(\alpha)} x^{\alpha-1}\, e^{-\beta x}\, \mathrm{d}x =$$

$$= \frac{\beta^\alpha}{\Gamma(\alpha)} \left(\int_0^\infty y^{\alpha-1}\, e^{-y}\, \mathrm{d}y\right) \frac{1}{\beta^{\alpha-1}} \frac{1}{\beta} = 1$$

where between the first and second row we substituted $y = \beta x$ and we simplified using the

definition of Γ-function. To calculate the c.f. :

$$
\begin{aligned}
\varphi(k) &= \int_{\mathbb{R}+} e^{ikx} \frac{\beta^\alpha}{\Gamma(\alpha)} \, x^{\alpha-1} \, e^{-\beta x} \, \mathrm{d}x = \\
&= \int_{\mathbb{R}+} \frac{\beta^\alpha}{\Gamma(\alpha)} \, x^{\alpha-1} \, e^{-(\beta-ik)x} \, \mathrm{d}x = \\
&= \frac{\beta^\alpha}{s^\alpha} \frac{1}{\Gamma(\alpha)} \int_{\mathbb{R}+} s^\alpha \, x^{\alpha-1} \, e^{-sx} \, \mathrm{d}x = \\
&= \frac{\beta^\alpha}{(\beta-it)^\alpha} = \\
&= \left(1 - i\frac{k}{\beta}\right)^{-\alpha}
\end{aligned}
$$

where in the third row we used the substitution $s = \beta - it$ while multiplying by s^α/s^α and the definition of Γ-function in the fourth row.

Exercise 3: C.F. of a general gaussian distribution

Given a random variable x drawn from a gaussian distribution $\mathcal{N}(\mu, \sigma^2)$, calculate its c.f. Remember that such distribution is defined as

$$
\mathcal{N}(\mu, \sigma^2) = \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}}
$$

Sol. Let's start from reconducting ourselves to the already known formula for the characteristic function of a gaussian distribution of mean $\mu = 0$ and conclude from that:

$$
\begin{aligned}
\varphi(k) &= \int_{\mathbb{R}} e^{ikx} \mathcal{N}_x(\mu, \sigma^2) \, \mathrm{d}x = \\
&= \int_{\mathbb{R}} e^{ikx} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \, \mathrm{d}x = \\
&= \int_{\mathbb{R}} e^{iky} e^{ik\mu} \frac{1}{\sqrt{2\pi\sigma^2}} e^{-\frac{y^2}{2\sigma^2}} \, \mathrm{d}y = \\
&= e^{ik\mu} \int_{\mathbb{R}} e^{iky} \mathcal{N}_y(0, \sigma^2) \, \mathrm{d}y = \\
&= e^{ik\mu} \, e^{-\frac{k^2\sigma^2}{2}}
\end{aligned}
$$

where we used the already mentioned equation 1.6 in the last passage and a substitution $y = x - \mu$ in the previous one.

Exercise 4

Write down the exponent of the example problem in matrix product notation and find $\mathbf{A}$.

Sol. We know that $-\frac{1}{2}\vec{x}^\mathsf{T}\mathbf{A}\vec{x} = -\frac{3}{2}(x_1^2 + x_2^2) + x_1 x_2$, so we can say that

$$
\begin{aligned}
\vec{x}^\mathsf{T}\mathbf{A}\vec{x} &= \sum_{i=1}^{2}\sum_{j=1}^{2} x_i \, \mathbf{A}_{ij} \, x_i = \\
&= x_1^2 \, \mathbf{A}_{11} + x_2^2 \, \mathbf{A}_{22} + x_1 \, x_2 \, \mathbf{A}_{12} + x_2 \, x_1 \, \mathbf{A}_{21} = \\
&= 3x_1^2 + 3x_2^2 - 2x_1 x_2
\end{aligned}
$$

By doing some intuitive matching and assuming $\mathbf{A}$ to be symmetric we can say that

$$
\mathbf{A} = \begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix}
$$

Exercise 5

Show that

$$\iint_{\mathbb{R}^2} \mathrm{d}x_1\, \mathrm{d}x_2\, e^{\left(-\frac{3}{2}(x_1^2+x_2^2)+x_1 x_2\right)} = \frac{\pi}{\sqrt{2}}$$

Sol. From the previous exercise, we saw the actual form of $\mathbf{A}$. We can now translate the request in the form of equation 1.7 and the results stems directly from applying equation 1.8, after calculating $\det(\mathbf{A}) = 8$.

$$Z(\mathbf{A}) = \frac{(2\pi)^{n/2}}{\sqrt{\det(\mathbf{A})}} = \frac{(2\pi)}{\sqrt{8}} = \frac{\pi}{\sqrt{2}}$$

Exercise 6

Let

$$p(x,y) = \frac{\sqrt{\det(\mathbf{A})}}{2\pi} e^{-\frac{1}{2} a_{11} x^2 + 2 a_{12} xy + a_{22} y^2}$$

where

$$\mathbf{A} = \begin{pmatrix} a_{11} & a_{12} \\ a_{21} & a_{22} \end{pmatrix}, \quad a_{11}, a_{22} > 0, \quad a_{12} = a_{21}$$

Show that $p(x,y)$ is normalized and that $\int p(x,y)\, \mathrm{d}y$ is still a gaussian PDF. Find the corresponding variance of the random variable x.

Sol. To show that $p(x,y)$ is normalized, we calculate

$$\int_{\mathbb{R}^2} \mathrm{d}x\, \mathrm{d}y\, p(x,y) = \frac{\sqrt{\det(A)}}{2\pi} \int_{\mathbb{R}^2} \mathrm{d}\vec{x}\, e^{-\frac{1}{2}\vec{x}^\mathsf{T} \mathbf{A} \vec{x}} = \frac{\sqrt{\det(A)}}{2\pi} Z(A) = 1$$

And we thus end the first request. To show that the marginalized probability is still a gaussian distribution and find its variance, we calculate explicitly the integral:

$$\int_{\mathbb{R}} p(x,y)\, \mathrm{d}y = \frac{\sqrt{\det(A)}}{2\pi} e^{-\frac{1}{2} a_{11} x^2} \int_{\mathbb{R}} \mathrm{d}y\, e^{-\frac{1}{2} a_{22} y^2 - a_{12}\, xy} =$$

$$= \frac{\sqrt{\det(A)}}{2\pi} e^{-\frac{1}{2} a_{11} x^2} \sqrt{\frac{2\pi}{a_{22}}}\, e^{\frac{a_{12}^2 x^2}{2 a_{22}}} =$$

$$= \sqrt{\frac{\det(A)}{2\pi\, a_{22}}} e^{-\frac{1}{2} x^2 \left(a_{11} - \frac{a_{12}}{a_{22}}\right)} =$$

$$= \mathcal{N}_x\left(0, \left(\frac{a_{22}}{a_{11} a_{22} - a_{12}^2}\right)\right) =$$

$$= \mathcal{N}_x\left(0, \frac{a_{22}}{\det(A)}\right)$$

Exercise 7

Do the calculations that leads to equation 1.12.

Sol. We want to evaluate the following

$$(-i)^2 \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} e^{-\frac{1}{2} \vec{k}^\mathsf{T} \mathbf{A}^{-1} \vec{k}}\bigg|_{\vec{k}=0}$$

To do so, we proceed step by step, starting from the derivative with respect to k_j:

$$\frac{\partial}{\partial k_j} \exp\left(-\frac{1}{2}\vec{k}^\mathsf{T} \mathbf{A}^{-1}\vec{k}\right) =$$

$$= \frac{\partial}{\partial k_j} \exp\left(-\frac{1}{2}\sum_{m,n} k_m \, \mathbf{A}^{-1}_{mn} \, k_n\right) =$$

$$= \frac{\partial}{\partial k_j} \exp\left[-\frac{1}{2}\left(\sum_{m\neq j, n\neq j} k_m \, \mathbf{A}^{-1}_{mn} \, k_n + \sum_{n\neq j} k_j \, \mathbf{A}^{-1}_{jn} \, k_n + \sum_{m\neq j} k_m \, \mathbf{A}^{-1}_{mj} \, k_j + k_j^2 \, \mathbf{A}^{-1}_{jj}\right)\right] =$$

$$= \frac{\partial}{\partial k_j} \exp\left[-\frac{1}{2}\left(\sum_{m\neq j, n\neq j} k_m \, \mathbf{A}^{-1}_{mn} \, k_n\right) - \frac{1}{2}\left(2\sum_{n\neq j} k_j \, \mathbf{A}^{-1}_{jn} \, k_n + k_j^2 \, \mathbf{A}^{-1}_{jj}\right)\right] =$$

$$= \exp\left[-\frac{1}{2}\left(\sum_{m\neq j, n\neq j} k_m \, \mathbf{A}^{-1}_{mn} \, k_n\right)\right] \frac{\partial}{\partial k_j} \exp\left[-\frac{1}{2}\left(2\sum_{n\neq j} k_j \, \mathbf{A}^{-1}_{jn} \, k_n + k_j^2 \, \mathbf{A}^{-1}_{jj}\right)\right] =$$

$$= \exp\left(-\frac{1}{2}\vec{k}^\mathsf{T} \mathbf{A}^{-1}\vec{k}\right)\left[-\frac{1}{2}\left(2\sum_{n\neq j} \mathbf{A}^{-1}_{jn} \, k_n + 2 k_j \, \mathbf{A}^{-1}_{jj}\right)\right] =$$

$$= \left(-\sum_n \mathbf{A}^{-1}_{jn} \, k_n\right) \exp\left(-\frac{1}{2}\vec{k}^\mathsf{T} \mathbf{A}^{-1}\vec{k}\right)$$

where in the fourth line we used the symmetricity of $\mathbf{A}$ (which implies the symmetricity of $\mathbf{A}^{-1}$). We can now proceed with the other derivative, recycling the results obtained just now, and the evaluation at 0:

$$(i^2)\frac{\partial}{\partial k_i}\left[\left(-\sum_n \mathbf{A}^{-1}_{jn} \, k_n\right) e^{-\frac{1}{2}\vec{k}^\mathsf{T} \mathbf{A}^{-1}\vec{k}}\right]\Bigg|_{\vec{k}=0} = -e^{-\frac{1}{2}\vec{k}^\mathsf{T} \mathbf{A}^{-1}\vec{k}}\left[-\mathbf{A}^{-1}_{ij} - \sum_n \mathbf{A}^{-1}_{mi} \, k_m\right]\Bigg|_{\vec{k}=0} = -\mathbf{A}^{-1}_{ij}$$

Exercise 8

From the previous case, show with the help of *Wick's theorem* that:

1. $\langle x_1^2 \, x_2^2\rangle = \frac{11}{64}$

2. $\langle x_1^4\rangle = 3\left(\frac{3}{8}\right)^2 = \langle x_2^4\rangle$

3. $\langle x_1 \, x_2^2\rangle = 0$

Sol.

1.

$$\langle x_1^2 \, x_2^2\rangle = \langle x_1 \, x_1\rangle \langle x_2 \, x_2\rangle + \langle x_1 \, x_2\rangle \langle x_1 \, x_2\rangle + \langle x_1 \, x_2\rangle \langle x_1 \, x_2\rangle = \frac{3}{8}\cdot\frac{3}{8} + \frac{1}{8}\cdot\frac{1}{8} + \frac{1}{8}\cdot\frac{1}{8} = \frac{11}{64}$$

2.

$$\langle x_1^4\rangle = \langle x_1 \, x_1\rangle \langle x_1 \, x_1\rangle + \langle x_1 \, x_1\rangle \langle x_1 \, x_1\rangle + \langle x_1 \, x_1\rangle \langle x_1 \, x_1\rangle = 3\langle x_1 \, x_1\rangle^2 = 3\cdot\left(\frac{3}{8}\right)^2 = \frac{27}{64}$$

Giving that $\langle x_1^2\rangle = \langle x_2^2\rangle$ in this particular instance, the second part of the equation naturally holds true.

3. Given that we're now dealing with an odd number of pairs, Wick's Theorem cannot be applied and remembering that the gaussian integrals over odd powers of one of the variables is null (due to it being the integral of an odd function over a symmetrical domain), we can safely say that the results is in fact 0.

> **Exercise 9: Exercises on sum of iid r.v.s**
>
> Calculate the distribution of $x = x_1 + x_2$ if x_1, x_2 are iids drawn from:
>
> 1. a uniform distribution $U([0,1])$;
>
> 2. a gaussian distribution $\mathcal{N}_x(\mu, \sigma)$;
>
> 3. an exponential distribution $q(x) = \lambda e^{-\lambda x}$

Sol.

1. One possibility to solve such integral is to observe that $U(x-t)$ is to 1 in $0 < x-t < 1$ and $U(t)$ is 1 in $0 < t < 1$. Graphing such values we obtain figure 4.1 We can now integrate
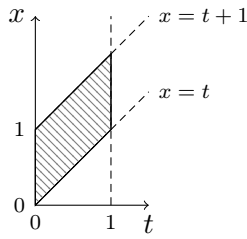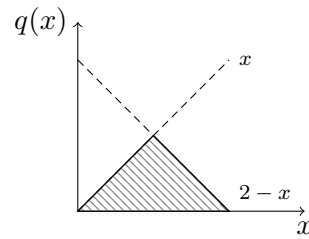

Fig. 4.1: Graph of the product $U(x-t)U(t)$ **Fig. 4.2:** Graph of the solution

over t, dividing the plane at $x = 1$:

$$x \in [0,1]: \; q(x) = \int_{\mathbb{R}} dt \, U(x-t)\, U(t) = \int_0^x dt = x \tag{4.1}$$

$$x \in [1,2]: \; q(x) = \int_{\mathbb{R}} dt \, U(x-t)\, U(t) = \int_{x-1}^1 dt = 2 - x \tag{4.2}$$

$$\Rightarrow q(x) = \begin{cases} x & \text{if } x \in [0,1] \\ 2 - x & \text{if } x \in [1,2] \end{cases} \tag{4.3}$$

2. It's known that the C.F. of a gaussian distribution $\mathcal{N}_x(\mu, \sigma^2)$ is the following:

$$\varphi_{\mu,\sigma^2}(k) = e^{ik\mu}\, e^{-\frac{\sigma^2 k^2}{2}} \tag{4.4}$$

Knowing that the distribution of a sum of i.i.d. r.v. can be computed through the product between characteristic functions, we calculate

$$\varphi(k) = \varphi_1(k)\, \varphi_2(k) = \tag{4.5}$$

$$= \left(e^{ik\mu}\, e^{-\frac{\sigma^2 k^2}{2}} \right)^2 = \tag{4.6}$$

$$= e^{ik(2\mu)}\, e^{-\frac{(\sqrt{2}\sigma)^2 k^2}{2}} \tag{4.7}$$

which is the C.F. of $\mathcal{N}_x(2\mu, \sqrt{2}\sigma^2)$

3. We can rewrite the exponential distribution, defined for positive values, in the following way:

$$q(x) = \lambda e^{-\lambda x}|x \in \mathbb{R}^+ = \Theta(x)\lambda e^{-\lambda x}|x \in \mathbb{R} \tag{4.8}$$

where Θ represent the Heaviside function. From this, we use the definition of convolution:

$$p(x) = \int_{\mathrm{Dom}_y} q_1(x - y)\, q_2(y)\, \mathrm{d}y = \tag{4.9}$$

$$= \int_{\mathbb{R}} [\Theta(x - y)\, \lambda e^{-\lambda(x-y)}]\, [\Theta(y)\, \lambda e^{-\lambda y}]\, \mathrm{d}y = \tag{4.10}$$

$$= \lambda^2 e^{-\lambda x} \int_{\mathbb{R}} \Theta(x - y)\, \Theta(y)\, \mathrm{d}y \tag{4.11}$$

If we now look at the content of the integral in last line, $\Theta(x - y)\Theta(y)$ is equal to 1 when $y \in [0, x]$ and 0 elsewhere, so the results is:

$$p(x) = x\lambda^2 e^{-\lambda x} \tag{4.12}$$

Exercise 10

Calculate the distribution of $x = x_1 \cdot x_2$ if x_1, x_2 are two positive i.i.d. r.v.

Sol. Similarly to what was done during the lectures for the sum of two i.i.d. r.v., we can show the following (where q_1, q_2 are the distributions from which x_1, x_2 are drawn):

$$q(x) = \int_0^\infty \delta(x - (x_1 x_2))\, q(x_1)\, q(x_2)\, \mathrm{d}x_1\, \mathrm{d}x_2 = \tag{4.13}$$

$$(y = \tfrac{x}{x_1} \to) = \int_\infty^0 \delta\left(x - \frac{x}{y}x_2\right) q\left(\frac{x}{y}\right) q(x_2) \left(-\frac{x}{y^2}\, \mathrm{d}y\right) \mathrm{d}x_2 = \tag{4.14}$$

$$= \int_0^\infty \delta\left[\frac{x}{y}(y - x_2)\right] q\left(\frac{x}{y}\right) q(x_2)\frac{x}{y^2}\, \mathrm{d}y\, \mathrm{d}x_2 = \tag{4.15}$$

$$= \int_{\mathbb{R}^+} \left|\frac{y}{x}\right| q\left(\frac{x}{y}\right) q(y)\frac{x}{y^2}\, \mathrm{d}y = \tag{4.16}$$

$$= \int_{\mathbb{R}^+} \frac{1}{|y|} q\left(\frac{x}{y}\right) q(y)\, \mathrm{d}y \tag{4.17}$$

where in between the third and fourth line, the properties of the Dirac delta were used. As for the C.F, not much else can be said other than the following:

$$\varphi(k) = \int_{\mathbb{R}^+} \mathrm{d}x \int_{\mathbb{R}^+ \times \mathbb{R}^+} \mathrm{d}x_1\, \mathrm{d}x_2\, q(x_1)\, q(x_2)\, e^{ikx}\, \delta(x - x_1 x_2) = \tag{4.18}$$

$$= \int_{\mathbb{R}^+ \times \mathbb{R}^+} \mathrm{d}x_1\, \mathrm{d}x_2\, q(x_1)\, q(x_2)\, e^{ikx_1x_2} \tag{4.19}$$

Exercise 11

Calculate the distribution of $x = x_1 + x_2 + \cdots + x_n$ if $x_1, x_2, \ldots, x_n$ are n independent but not identically distributed r.v.

Sol. Remembering that the distribution of n independent r.v. (without specifying the domain to lighten the notation) can be calculated as

$$q(x) = \int \delta\left(x - \sum_{i=1}^n x_i\right) \prod_{i=1}^n (q_i(x_i)\, \mathrm{d}x_i) \tag{4.20}$$

We can obtain the wanted C.F. as follows:

$$\varphi(k) = \int q(x)e^{ikx}\,\mathrm{d}x = \tag{4.21}$$

$$= \int \delta\left(x - \sum_{i=1}^{n} x_i\right)\left(\prod_{i=1}^{n} q_i(x_i)\,\mathrm{d}x_i\right)e^{ikx}\,\mathrm{d}x = \tag{4.22}$$

$$= \int \left(\prod_{i=1}^{n} q_i(x_i)\,\mathrm{d}x_i\right)e^{ik\left(\sum_{i=1}^{n} x_i\right)} = \tag{4.23}$$

$$= \int \prod_{i=1}^{n} q_i(x_i)\,\mathrm{d}x_i\, e^{ikx_i} = \tag{4.24}$$

$$= \prod_{i=1}^{n} \int q_i(x_i)\,\mathrm{d}x_i\, e^{ikx_i} = \tag{4.25}$$

$$= \prod_{i=1}^{n} \varphi_i(k) \tag{4.26}$$

Exercise 12

Show why only $-\frac{k^2}{2n}$ remains for the exponent.

Sol.

Exercise 13: Exercises on Central Limit Theorem

Show that

1. $\sum_{i=1}^{n} x_i \sim \mathcal{N}(n\mu, n\sigma^2)$;

2. $\frac{1}{n}\sum_{i=1}^{n} x_i \sim \mathcal{N}(\mu, \frac{\sigma^2}{n})$

Sol.

Exercise 14: Better Laplace method approximation

Show that a better approximation is given by

$$I(\lambda) \simeq e^{\lambda f(x_0)}\sqrt{\frac{2\pi}{\lambda\,|f''(x_0)|}}\left(g(x_0) + \frac{c}{\lambda}\right) \qquad as\ \lambda \to +\infty$$

where c is a constant that depends on derivatives of $f(x)$ up to 4th order (at $x = x_0$) and on $g(x_0)$, $g'(x_0)$ and $g''(x_0)$.

Sol.

Exercise 15: Better modified Bessel function approximation

Show that a better approximation is given by

$$k_\nu(x) \simeq e^{-x}\sqrt{\frac{\pi}{2x}}\left(1 + \frac{c(\nu)}{x}\right) \qquad as\ \lambda \to +\infty$$

and calculate $c(\nu) = \frac{4\nu^2 - 1}{8}$.

Sol.

Exercise 16: Demonstration of Gamma function and factorial relation

Show that $\Gamma(\lambda+1) = \lambda\Gamma(\lambda)$, hence $\lambda! = \Gamma(\lambda+1)$ which generalize the factorial to real (and complex) numbers.

Sol.

Exercise 17

Verify the following for large λ

1. $I(\lambda) = \int_0^\infty e^{-\lambda t} e^{-\frac{1}{t}} \, \mathrm{d}t \simeq \dfrac{\sqrt{\pi} e^{-2\sqrt{\lambda}}}{\lambda^{\frac{3}{4}}}$ (Application of Stirling's Formula)

2. $I(\lambda) = \int_{-2}^0 e^t e^{\lambda(3t^2+2t^3)} \, \mathrm{d}t \approx e^{\lambda-1} \sqrt{\dfrac{\pi}{3\lambda}}$

3. $I(\lambda) = \int_0^1 e^t e^{\lambda(3t^2+2t^3)} \, \mathrm{d}t \approx e^{5\lambda+1} \dfrac{1}{12\lambda}$

4. $I(\lambda) = \int_0^1 \sqrt{t+1} e^{\lambda(2t-t^2)} \, \mathrm{d}t \approx e^\lambda \sqrt{\dfrac{\pi}{2\lambda}}$

5. $I(\lambda) = \int_{-2}^0 (1+t^2) e^{\lambda(t^3-1)} \, \mathrm{d}t \approx 5e^{6\lambda} \dfrac{1}{12\lambda}$

Sol.

4.2   Chapter 2: Deterministic Reaction Dynamics

Exercise 18: Special case: equal concentrations

Solve the logistic equation (2.5) in the critical case $c = 0$. What is the interpretation in term of reagents and products?

Sol.
The equation we want to solve becomes

$$\dot{x} = -kx^2$$

with initial condition $x(0) = x_0$. This also can be done by separation of variables:

$$\dot{x} = \frac{\mathrm{d}x}{\mathrm{d}t} = -k\,x^2$$

$$\frac{\mathrm{d}x}{-x^2} = k\,\mathrm{d}t$$

$$\int\left(-\frac{1}{x^2}\right)\mathrm{d}x = \int k\,\mathrm{d}t$$

$$\frac{1}{x} = k\,t + q$$

$$x = \frac{1}{k\,t + q}$$

$$\text{for } x(0) = x_0 \quad x(0) = \frac{1}{q} = x_0 \qquad q = \frac{1}{x_0}$$

$$x(t) = \frac{x_0}{1 + x_0\,k\,t} \xrightarrow{t\to+\infty} 0$$

$$c = x(t) - y(t) = 0 \quad\Longrightarrow\quad x(t) = y(t) = \frac{x_0}{1 + x_0\,k\,t} \xrightarrow{t\to+\infty} 0$$

$$\text{if } x(t) + z(t) = C \quad\Longrightarrow\quad z(t) = C - x(t) \xrightarrow{t\to+\infty} C = x_0 + z_0$$

In this case, if the concentrations of reactant are the same at the start, they will both be consumed at the end and the product will increase by the same quantity. The final concentration of the product is equal to that of the reactant, plus its initial concentration.

Exercise 19: Solution of the reversible equation for X

The equation (2.9) can also be solved analitically. Do it.

Sol.

The equation

$$\dot{x} = k_+ x(c_1 - x) + k_-(c_2 - x)$$

$$\text{from:} \qquad X + Y \underset{k_-}{\overset{k_+}{\rightleftharpoons}} Z$$

$$\text{and} \qquad c_1 = x(t) - y(t) = x(0) - y(0)$$

$$c_2 = x(t) + z(t) = x(0) + z(0) > 0$$

can also be solved by separation of variables

$$\dot{x} = \frac{\mathrm{d}x}{\mathrm{d}t} = k_+ x(c_1 - x) + k_-(c_2 - x)$$

$$\frac{\mathrm{d}x}{k_+ x(c_1 - x) + k_-(c_2 - x)} = \mathrm{d}t \qquad \frac{\mathrm{d}x}{k_+(c_1\,x - x^2 + k\,c_2 - k\,x)} = \mathrm{d}t \quad \text{for } k = \frac{k_-}{k_+}$$

$$\frac{\mathrm{d}x}{-x^2 + (c_1 - k)x + k\,c_2} = k_+\,\mathrm{d}t$$

using the partial fraction decomposition for the denominator

$$\frac{1}{-x^2 + (c_1 - k)x + k\,c_2} = \frac{1}{-(x - \omega_1)(x - \omega_2)}$$

$$\text{for} \quad \omega_{1,2} = \frac{(c_1 - k) \pm \sqrt{(c_1 - k)^2 + 4k\,c_2}}{2} = \frac{c_1 - k}{2}\,(1 \pm R)\,, \quad R \equiv \sqrt{1 + \frac{4k\,c_2}{(c_1 - k)^2}}$$

$$\frac{1}{(\omega_1 - x)(x - \omega_2)} = \frac{A}{\omega_1 - x} + \frac{B}{x - \omega_2}$$

$$\text{for} \quad A(x - \omega_2) + B(\omega_1 - x) = 1 \quad \begin{cases} A\,x - B\,x = 0 \\ -A\omega_2 + B\omega_1 = 1 \end{cases} \quad \begin{cases} A = B \\ A(\omega_1 - \omega_2) = 1 \end{cases}$$

$$A = \frac{1}{\omega_1 - \omega_2} = \frac{1}{R(c_1 - k)}$$

it is now possible to integrate

$$\int \left(\frac{1}{\omega_1 - x} + \frac{1}{x - \omega_2} \right) \mathrm{d}x = \int R(c_1 - k)k_+ \,\mathrm{d}t$$

$$-\ln\,(\omega_1 - x) + \ln\,(x - \omega_2) = \ln\left(\frac{x - \omega_2}{\omega_1 - x} \right) = R(c_1 - k)k_+\,t + q$$

$$\frac{x - \omega_2}{\omega_1 - x} = C\,e^{R(c_1 - k)k_+\,t}$$

$$x(1 + C\,e^{R(c_1 - k)k_+\,t}) = C\,\omega_1 e^{R(c_1 - k)k_+\,t} - \omega_2$$

$$x(t) = \frac{C\,\omega_1 e^{R(c_1 - k)k_+\,t} - \omega_2}{1 + C\,e^{R(c_1 - k)k_+\,t}}$$

$$\text{imposing } x(0) = x_0, \qquad x(0) = \frac{C\,\omega_1 - \omega_2}{1 + C} = x_0 \qquad C = \frac{x_0 + \omega_2}{\omega_1 - x_0}$$

$$\text{noticing } R(c_1 - k) = \omega_1 - \omega_2 \qquad x(t) = \frac{(x_0 + \omega_2)\omega_1 e^{(\omega_1 - \omega_2)k_+\,t} - (\omega_1 - x_0)\omega_2}{(\omega_1 - x_0) + (x_0 + \omega_2)e^{(\omega_1 - \omega_2)k_+\,t}}$$

Exercise 20: Analysis of conservation laws

For the equation (2.10) at stationarity $\frac{x\,y^3}{z^2} = \frac{k_-}{k_+}$, but there are also some conservation laws:

$$3x(t) - y(t) = c_1, \qquad 2x(t) + z(t) = c_2, \qquad 2y(t) + 3z(t) = c_3$$

why are these quantities conserved and why are c_1, c_2, c_3 not independent?

Sol.
Watching equations (2.10) and (2.11) it is possible to se that the direct reaction occur only when 1 unit of X interacts with 3 units of Y, producing 2 units of Z; at the same time the backward reaction happens only with the collision of 2 Z units and produce 3 units of Y and 1 of X. The stoichiometric proportions are conserved for the whole process, so it is coherent to obtain those relation in the conservation laws.
For the practicle derivation, it easy to check that the equation from (2.11) satisfy:

$$3\,\dot{x} = \dot{y} \qquad 2\,\dot{x} = -\dot{z} \qquad 2\,\dot{y} = -3\,\dot{z}$$

and from their integration in range $[0; t]$ the 3 conservation laws can be derived.
Giving the definition of c_1, c_2, c_3 is also trivial to check that they are linear dependent, connected through the identity

$$3\,c_2 - 2\,c_1 = c_3$$

Exercise 21: General binary reversible equation analysis

Calculate the conserved quantities for the equation (2.12) using the corresponding ODEs.

Sol.
The corresponding ODEs are

$$
\begin{cases}
\dot{x} = a\left(-k_+\, x^a\, y^b + k_-\, z^c\, w^d\right) \\
\dot{y} = b\left(-k_+\, x^a\, y^b + k_-\, z^c\, w^d\right) \\
\dot{z} = c\left(+k_+\, x^a\, y^b - k_-\, z^c\, w^d\right) \\
\dot{w} = d\left(+k_+\, x^a\, y^b - k_-\, z^c\, w^d\right)
\end{cases}
$$

it is easy to see that apart of stoichiometric coefficient, $\dot{x} \sim \dot{y} \sim -\dot{z} \sim -\dot{w}$

$$
\frac{\dot{x}}{a} = \frac{\dot{y}}{b} \Rightarrow b\,\dot{x} = a\,\dot{y} \qquad b\int_0^t \dot{x} = a\int_0^t \dot{y} \quad \Rightarrow b\left(x(t) - x(0)\right) = a\left(y(t) - y(0)\right)
$$

$$
\frac{\dot{z}}{c} = \frac{\dot{w}}{d} \Rightarrow d\,\dot{z} = c\,\dot{w} \qquad d\int_0^t \dot{z} = c\int_0^t \dot{w} \quad \Rightarrow d\left(z(t) - z(0)\right) = c\left(w(t) - w(0)\right)
$$

$$
\frac{\dot{x}}{a} = -\frac{\dot{z}}{c} \Rightarrow c\,\dot{x} = -a\,\dot{z} \qquad c\int_0^t \dot{x} = -a\int_0^t \dot{z} \Rightarrow c\left(x(t) - x(0)\right) = -a\left(z(t) - z(0)\right)
$$

from which is possible to find the conservation laws:

$$
\begin{aligned}
b\,x(t) - a\,y(t) &= c_1 = b\,x(0) - a\,y(0) \\
d\,z(t) - c\,w(t) &= c_2 = d\,z(0) - c\,w(0) \\
c\,x(t) + a\,z(t) &= c_3 = c\,x(0) + a\,z(0)
\end{aligned}
$$

Exercise 22: Reaction rate for water

For the reversible reaction described by the well known equation, presented at the beginning of this chapter:

$$
2H_2 + O_2 \underset{k_-}{\overset{k_+}{\rightleftharpoons}} 2H_2O
$$
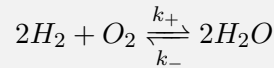
1. write down the ODEs for the rate equation

2. calculate the conservation laws and the stationary values of the concentrations starting from $x_0 = 2y_0$ and $z_0 = 0$

3. solve the final equation when $k_+ = k_-$ and $x_0 = 1$ (mol).

Sol.
1. using x, y, z for concentrations of H_2, O_2, H_2O respectively and the law of mass action it is easy to find out

$$
\begin{cases}
\dot{x} = 2\left(-k_+ x^2\, y + k_- z^2\right) \\
\dot{y} = -k_+ x^2\, y + k_- z^2 \\
\dot{z} = 2\left(k_+ x^2\, y - k_- z^2\right)
\end{cases}
$$

2. seeing the structure of the ODEs is similar, it is easy to demonstrate that

$$
\begin{aligned}
\dot{x} = 2\dot{y} \qquad & x(t) - x(0) = 2\,y(t) - 2\,y(0) \qquad & x(t) - 2\,y(t) = c_1 = x_0 - 2\,y_0 = 2\,y_0 - 2\,y_0 = 0 \\
\dot{x} = -\dot{z} \qquad & x(t) - x(0) = -z(t) + z(0) \qquad & x(t) + z(t) = c_2 = x_0 + z_0 = 2\,y_0 + 0 = 2\,y_0
\end{aligned}
$$

For a stationary state defined by the concentrations $\bar{x}, \bar{y}, \bar{z}$ the conditions to be met are

$$\begin{cases} \dot{x} = 2\left(-k_+\bar{x}^2\,\bar{y} + k_-\bar{z}^2\right) = 0 \\ \dot{y} = -k_+\bar{x}^2\,\bar{y} + k_-\bar{z}^2 = 0 \\ \dot{z} = 2\left(k_+\bar{x}^2\,\bar{y} - k_-\bar{z}^2\right) = 0 \end{cases}$$

using the first and adding the conservation laws to simplify it becomes

$$x(t) - 2\,y(t) = \bar{x} - 2\,\bar{y} = c_1 = 0 \qquad \bar{y} = \frac{1}{2}\bar{x}$$

$$x(t) + z(t) = \bar{x} + \bar{z} = c_2 = x_0 \qquad \bar{z} = x_0 - \bar{x}$$

$$0 = \dot{x} = 2\left(-k_+\bar{x}^2\,\bar{y} + k_-\bar{z}^2\right) = -k_+\bar{x}^2\,\bar{x} + 2\,k_-\,(x_0 - \bar{x})^2$$

$$-k_+\bar{x}^3 + 2\,k_-\left(\bar{x}^2 + x_0^2 - 2\,x_0\bar{x}\right) = -k_+\bar{x}^3 + 2\,k_-\,\bar{x}^2 - 4\,k_-\,x_0\bar{x} + 2\,k_-\,x_0^2 = 0$$

$$\text{for } k = \frac{k_-}{k_+} \qquad 0 = \bar{x}^3 - 2\,k\,\bar{x}^2 + 4\,k\,x_0\,\bar{x} - 2\,k\,x_0^2$$

where one real solution is possible but not simple.
3. solving when $k_+ = k_- \Rightarrow k = 1$, $x_0 = 1$

$$\bar{x}^3 - 2\,\bar{x}^2 + 4\,\bar{x} - 2 = 0$$

this again has no easy solutions, and only one is real.

> **Exercise 23: Lotka Volterra equations' stability and conservation law**
>
> Show that at stationarity the concentrations assume the values
>
> $$\bar{x} = \frac{k_3}{k_2}, \qquad \bar{y} = \frac{k_1}{k_2}$$
>
> but the Jacobian at $(\bar{x}, \bar{y})$ has pure imaginary eigenvalues
>
> $$\lambda = \pm i\sqrt{k_1 k_3}$$
>
> Show that the following is a non-linear conserved quantity (a *conservation law*)
>
> $$V(x, y) = k_2(x + y) - k_3 \ln x - k_1 \ln y$$

Sol.
The Lotka-Volterra equations shown in (2.14) may admit a stationarity state for concentrations $\bar{x}, \bar{y}$ where the null derivative conditions are met

$$\begin{cases} \dot{x} = k_1\,\bar{x} - k_2\,\bar{x}\,\bar{y} = 0 \\ \dot{y} = k_2\,\bar{x}\,\bar{y} - k_3\,\bar{y} = 0 \end{cases} \longrightarrow \begin{cases} k_2\,\bar{x}\,\bar{y} = k_1\,\bar{x} \\ k_2\,\bar{x}\,\bar{y} - k_3\,\bar{y} = 0 \end{cases}$$

$$\text{if } \bar{x} \neq 0 \quad \begin{cases} \bar{y} = \frac{k_1}{k_2} \\ k_1\,\bar{x} = k_3\,\frac{k_1}{k_2} \end{cases} \longrightarrow \begin{cases} \bar{x} = \frac{k_3}{k_2} \\ \bar{y} = \frac{k_1}{k_2} \end{cases}$$

So the defined values correspond to those in the steady state, if the initial condition are not $x_0 = 0, y_0 = 0$, that are obviously stable but not interesting.
The Jacobian directly comes from the partial derivatives of the ODEs in (2.14), in the steady state assumes values of:

$$J(x,y) = \begin{pmatrix} k_1 - k_2\,y & -k_2\,x \\ k_2\,y & k_2\,x - k_3 \end{pmatrix} \qquad J(\bar{x},\bar{y}) = \begin{pmatrix} k_1 - k_2\,\frac{k_1}{k_2} & -k_2\,\frac{k_3}{k_2} \\ k_2\,\frac{k_1}{k_2} & k_2\,\frac{k_3}{k_2} - k_3 \end{pmatrix} = \begin{pmatrix} 0 & -k_3 \\ k_1 & 0 \end{pmatrix}$$

it is possible to directly calculate the eigenvalues by characteristic polynomial p_J

$$p_J(\lambda) = \det(J(\bar{x},\bar{y}) - \lambda\mathbb{1}) = \det \begin{pmatrix} -\lambda & -k_3 \\ k_1 & -\lambda \end{pmatrix} = 0$$

$$= \lambda^2 + k_1\,k_3 \quad \Rightarrow \quad \lambda_{1,2} = \pm i\sqrt{k_1\,k_3}$$

remembering that by definition $k_i > 0$. So $\bar{x},\bar{y}$ are the concentrations at stability but the Jacobian has pue imaginary eigenvalues.
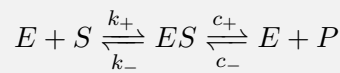In the phase space this equation defines a closed orbit, the stability point is neutrally stable. The neutral stability if defined for point in which proximity small perturbations only moves to the next near trajectory, in contrast with stability and instability, for which small perturbations leads to orbiting more and more close to the point (attractor) or far away from it respectively. The non-linear conserved quantity can be demonstrated by derivation and substitution with equations in (2.14)

$$V(x,y) = k_2(x + y) - k_3\ln x - k_1\ln y = \text{constant} \quad \Leftrightarrow \quad \frac{\mathrm{d}V(x,y)}{\mathrm{d}t} = 0$$

$$\frac{\mathrm{d}V(x,y)}{\mathrm{d}t} = k_2(\dot{x} + \dot{y}) - k_3\frac{\dot{x}}{x} - k_1\frac{\dot{y}}{y}$$

$$\stackrel{(2.14)}{=} k_2(k_1\,x - k_2\,x\,y + k_2\,x\,y - k_3\,y) - k_3\frac{k_1\,x - k_2\,x\,y}{x} - k_1\frac{k_2\,x\,y - k_3\,y}{y}$$

$$= k_2(k_1\,x - k_3\,y) - k_3(k_1 - k_2\,y) - k_1(k_2\,x - k_3)$$

$$= k_1\,k_2\,x - k_2\,k_3\,y - k_1\,k_3 + k_2\,k_3\,y - k_1\,k_2\,x + k_1\,k_3 = 0$$

the given equation is a conserved quantity, so can be seen as a non-linear conservation law.
The conserved quantity indicates the presence of something fishy: as useful as conservation laws may be in physics, they are unrealistic in biology. In this case it indicates that preys' concentration can go unreasonably low but they will eventually recover from that, waiting enough time; this is obviously unreal, because under a certain value the population will go extinct.
This can be a useful reminder when modeling biological systems: always pay attention to conservation laws, because they probability don't have a real counterpart.
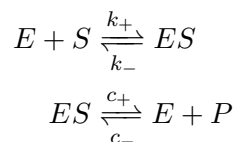

Exercise 24: Enzymatic reaction

Find the ODEs of the following enzymatic reaction:

$$E + S \underset{k_-}{\overset{k_+}{\rightleftharpoons}} ES \underset{c_-}{\overset{c_+}{\rightleftharpoons}} E + P$$

There are 4 dynamic variables whose reaction rates has to be described in this system, E, S, ES and P.

Sol.
For each variable is defined its concentration ([...]) as $[E] = x$, $[S] = y$, $[ES] = z$, $[P] = w$. The reaction can be decomposed into two separate reactions as

$$E + S \underset{k_-}{\overset{k_+}{\rightleftharpoons}} ES$$

$$ES \underset{c_-}{\overset{c_+}{\rightleftharpoons}} E + P$$

from which is possible to apply the law of mass action to write directly the ODEs

$$
\begin{cases}
\dot{x} = -k_+\, x\, y + k_-\, z + c_+\, z - c_-\, x\, w \\
\dot{y} = -k_+\, x\, y + k_-\, z \\
\dot{z} = k_+\, x\, y - k_-\, z - c_+\, z + c_-\, x\, w \\
\dot{w} = c_+\, z - c_-\, x\, w
\end{cases}
$$

where is also possible to identity some conservation laws:
$x(t) + z(t) = x(0) + z(0)$ and $x(t) - y(t) - w(t) = x(0) - y(0) - w(0)$.

Exercise 25: Brusselator equations

Derive the ODEs for X and Y from the following reactions:

$$A \xrightarrow{k_1} X$$

$$B + X \xrightarrow{k_2} Y + D$$

$$2X + Y \xrightarrow{k_3} 3X$$

$$X \xrightarrow{k_4} E$$
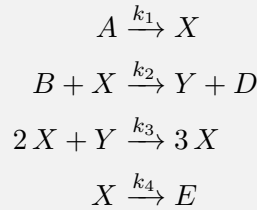
Only X and Y have to be considered as dynamic variables, as it is assumed concentrations of A, B, D and E remain constant and are in excess.
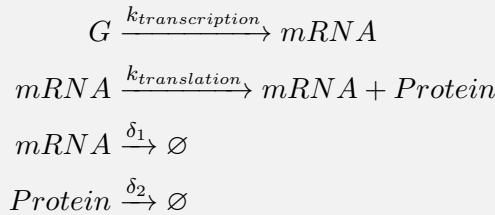

Sol.
Assuming x, y concentrations of species X, Y and applying the law of mass action

$$
\begin{cases}
\dot{x} = k_1 - k_2\, x + k_3\, x^2\, y - k_4\, x \\
\dot{y} = k_2\, x - k_3\, x^2\, y
\end{cases}
$$

noticing that the first reaction occur at a rate k_1 that does not depend on any dynamic variable, the first term of the ODE for x consist only of that, describing a constant increment independent from concentrations; in the third reaction only one unit of X is produced, thus no stoichiometric coefficient is needed in the corresponding element of the ODEs.

Exercise 26: Gene expression dynamics

$$G \xrightarrow{k_{transcription}} mRNA$$

$$mRNA \xrightarrow{k_{translation}} mRNA + Protein$$

$$mRNA \xrightarrow{\delta_1} \varnothing$$

$$Protein \xrightarrow{\delta_2} \varnothing$$

Derive the ODEs for $mRNA$ and $Protein$, the two dynamic variables in the previous eq.s.

Sol.
Through the law of mass action and remembering that G does not enter into the equations,

$$
\begin{cases}
\dot{mRNA} = k_{transcription} - \delta_1\, mRNA \\
\dot{Protein} = k_{translation}\, mRNA - \delta_2\, Protein
\end{cases}
$$

in the second reaction $mRNA$ acts like a reactant in excess, without being consumed nor produced, so this does not influence $mRNA$'s ODE.

> **Exercise 27: The SEIR model**
>
> Derive the ODEs for S, E, I and R from the following reactions:
>
> $$S + I \xrightarrow{\beta} E + I$$
> $$E \xrightarrow{\sigma} I$$
> $$I \xrightarrow{\gamma} R$$
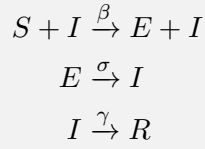
Sol.
Using a logical corresponding between dynamic variables (capital letters) and their concentrations (lowercase letters), from law of mass action
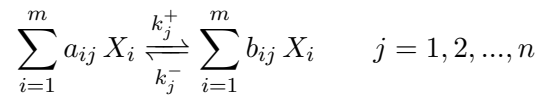
$$\begin{cases} \dot{s} = -\beta\, s\, i \\ \dot{i} = \sigma\, e - \gamma i \\ \dot{e} = \beta\, s\, i - \sigma\, e \\ \dot{r} = \gamma\, i \end{cases}$$

> **Exercise 28: Proof of general chemical equations ODEs**
>
> carefully prove the previous result: obtain (2.16) from (2.15)

Sol.
It is asked to derive the ODEs of the system of reactions summarized in

$$\sum_{i=1}^{m} a_{ij}\, X_i \underset{k_j^-}{\overset{k_j^+}{\rightleftharpoons}} \sum_{i=1}^{m} b_{ij}\, X_i \qquad j = 1, 2, ..., n$$

where are described n different equations for m different dynamic variables.
Every direct(reverse) reaction j occurs at a rate that can be expressed as

$$k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}}$$

$$k_j^- \prod_{i=1}^{m} x_i^{b_{ij}}$$

for x_i concentration of X_i, where every element that takes part in the reaction is multiplied, raised to the power corresponding to its stoichiometric coefficient.
Every reactions contributes to the variation of the concentration of each element via its stoichiometric coefficient, based on direction of the reaction and side in which the species appear: for the direct reaction, a species is decreased through coefficient a_{ij} and increased through b_{ij}, for the reverse reaction is increased through coefficient a_{ij} and decreased through b_{ij}.
The contribution for X_i from the reaction j is

$$\dot{x}_{i,j} = -a_{ij}\, k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}} + b_{ij}\, k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}} - b_{ij}\, k_j^- \prod_{i=1}^{m} x_i^{b_{ij}} + a_{ij}\, k_j^- \prod_{i=1}^{m} x_i^{b_{ij}}$$

$$= -(a_{ij} - b_{ij}) k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}} + (a_{ij} - b_{ij}) k_j^- \prod_{i=1}^{m} x_i^{b_{ij}}$$

keeping in mind that for every reaction a species X_i can be a reactant, a product, both or neither, depending on if its stoichiometric coefficient is non-zero and if it is different between the two

sides of the reaction. The contributions of various reaction must be added, and this is the case for each variable:

$$\forall i \in [0;m] \quad \dot{x}_i = \sum_{j=1}^{n} \left(-(a_{ij} - b_{ij}) \, k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}} + (a_{ij} - b_{ij}) \, k_j^- \prod_{i=1}^{m} x_i^{b_{ij}} \right)$$

$$= (b_{ij} - a_{ij}) \sum_{j=1}^{n} \left(k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}} - k_j^- \prod_{i=1}^{m} x_i^{b_{ij}} \right)$$

$$= (b_{ij} - a_{ij}) \sum_{j=1}^{n} r_j(\bar{x}) \quad \text{for } r_j(\bar{x}) = k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}} - k_j^- \prod_{i=1}^{m} x_i^{b_{ij}}$$

Bibliography

[1] Geoffrey Grimmett and David Stirzaker. *Probability and Random Processes.* Oxford University Press, 2020. ISBN: 9780198847595.