Notes for Models of Theoretical Physics

Models of Theoretical Physics

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Models of Theoretical Physics

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ODEs from reaction rates **First Semester**

Lecture 1

Date: 2025-10-17 Profesor: Azaele Sandro

0.1 ODEs from reaction rates

Chemical reactions form a broad field of applications where deterministic and stochastic methods are very useful. Such reactions include a wide class of systems where individuals of some entity encounter randomly and then react with some others of the same or different entity (reactants) and produce individuals which may be of a different nature (products) w.r.t. the reactants. The systems that can be studied in this framework include:

1. Actual chemical reactions which involve particles on molecules which transform upon collisions.
2. Population systems, where individuals may die, give birth, mate, consume each other, immigrate....
3. Epidemics, where diseases are transmitted from ind. to ind. (infected susceptibles)
4. Gene expression, where genes can be transcribed (into mRNA) and translated (into proteins) upon the appropriate occurrence of some transcription factors.
5. ...

These reactions may be reversible or not, according to whether the direct reaction can also occur in the backward direction.

In this part of the module we will be only concerned with the deterministic properties of these systems (mean-field approx.), namely, we will not study their stochastic properties.

We will write down the ODEs for the concentrations of the reactants and products starting from the corresponding rules that govern the chemical reactions.

0.1.1 Binary and irreversible reaction

A molecule of type X and a molecule of type Y (reactants) collide and react to produce a molecule of type Z (product):

$$x + y \xrightarrow{k} z \tag{0.1}$$

K is the kinetic constant which is used to compute $r(x, y)$, which gives the rate of occurrence of the reaction

$$2H_2 + O_2 \xrightarrow{K} 2H_2O \tag{0.2}$$

stoichiometric coefficients: # of react. or prod. of each type that are consumed or produced in the reaction.

0.1.2 Calculation of the reaction rate

We assume that the reaction occurs in a finite volume V where the molecules are well-stirred and the concentrations of X, Y and Z are "small", despite the number of molecules of each type is "large". We will assume that the concentrations $x = \frac{n_x}{v}, y = \frac{n_y}{v}, z = \frac{n_z}{v}$ (n_i : # of molec.

of type i) are continuous variables. We want to estimate $r(x, y)$, the reaction rate, in the diluted limit case:

$$r(x,y) \simeq r(0,0) + (\partial_x r_0)\, x + \left(\partial_y r_0\right) y + \left(\frac{1}{2}\partial^2_{xx} r_0\right) x^2 + \left(\partial^2_{xy} r_0\right) xy + \left(\frac{1}{2}\partial^2_{yy} r_0\right) y^2 + h_0 t \tag{0.3}$$

small concentrations x, y We expect that $r(0, y) = 0$ for all y as well as $r(x, 0) = 0$ for all x, because we need both x and y for the reaction to occur. Therefore from eq. (2) we get $r(0, y) = r(0, 0) + \left(\partial_y r_0\right) y + \left(\frac{1}{2}\partial^2_{yy} r_0\right) y^2 \equiv 0 \quad \Longrightarrow r(0, 0) = 0, \partial_y r_0 = 0, \partial^2_{yy} r_0 = 0\, r(0, x) = \partial_x r_0 x + \frac{1}{2}\partial^2_{xx} r_0 x^2 \equiv 0 \Longrightarrow \partial_x r_0 = 0, \partial^2_{xx} r_0 = 0$ Hence we are left with

$$r(x, y) = \partial^2_{xy} r_0 xy \equiv kxy \tag{0.4}$$

Obs: particles are free to move and randomly meet with each other: the prob. of x and y to collide are indip. When they meet, they can react. where the kinetic constant k does not depend on concentrations. k may depend on the temperature, $k = k_0 e^{-\frac{E}{kT}}$ (E activation energy), with the Arrhenius factor $e^{-E/kT}$.

The previous motivation leads to an approximate/empirical "law" which is simple and useful in many situations:

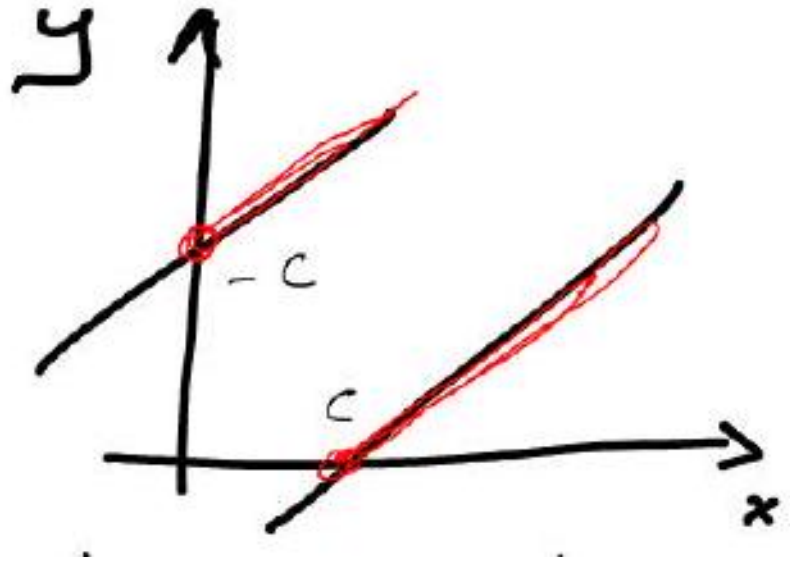
The law of Mass Action

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

We can use this law to deduce the ODEs for the evolution of the concentrations. If we know the concent. at time t, then at time $t + \Delta t$ (see eq.(1)):

$$\begin{aligned} x(t+\Delta t) &= x(t) - kx(t)y(t)\Delta t \\ y(t+\Delta t) &= y(t) - kx(t)y(t)\Delta t \\ z(t+\Delta t) &= z(t) + kx(t)y(t)\Delta t \end{aligned} \quad \xrightarrow{\Delta t \to 0} \quad \begin{cases} \dot{x} = -kxy, x(0) = x_0 \\ \dot{y} = -kxy, y(0) = y_0 \\ \dot{z} = kxy, z(0) = z_0 \end{cases} \tag{0.5}$$

Eq. (4) has a conservation law: $\dot{x} - \dot{y} = 0 \quad \Longrightarrow \quad x(t) - y(t) = x_0 - y_0 = c$ constant Therefore we can simplify eq. (4):



$$\dot{x} = -kx(x-c) = kx(c-x) \tag{0.6}$$

This is called logistic equation and can be solved analytically:

$$x(t) = \frac{cx_0e^{ckt}}{c + x_0\left(e^{ckt} - 1\right)} \tag{0.7}$$

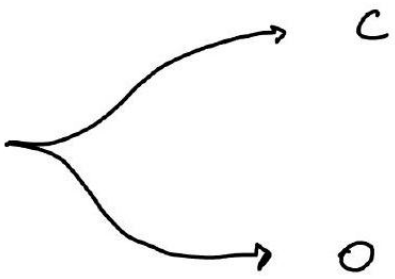
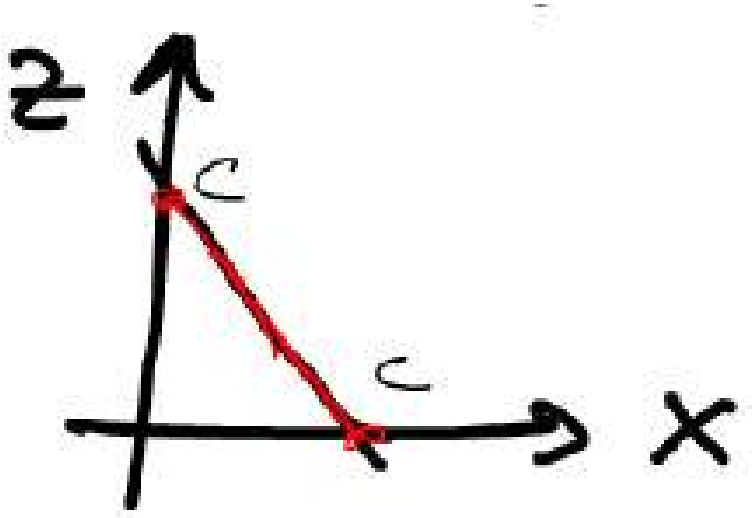


Figure 1: if $c > 0$ as $t \to +\infty$

if $c < 0$

Check of (6) out. What happens if $c = 0$? Solve eq. (4) for $z(t)$. There is another independent conservation law: $\dot{x} + \dot{z} = 0 \Rightarrow x(t) + z(t) = x_0 + z_0$ Therefore if $c > 0, z \longrightarrow x_0 + z_0 - c = z_0 + y_0$ as $t \to \infty$; all y goes to z. If $c < 0, z \to z_0 + x_0$.



0.1.3 Binary reversible reaction:

$$x + y \underset{k_-}{\overset{k_+}{\rightleftarrows}} z \quad k_\pm > 0 \tag{0.8}$$

Along the same lines as before we deduce the evolution of concent.

$$\begin{cases} \dot{x} = k_- z - k_+ xy \\ \dot{y} = k_- z - k_+ xy \\ \dot{z} = -k_- z + k_+ xy \end{cases} \tag{0.9}$$

Verify that there are two independent conservation laws $x(t) - y(t) = c_1$, and $x(t) + z(t) = c_2$. Hence the eq. for x can be written as

$$\dot{x} = k_+ x\,(c_1 - x) + k_-\,(c_2 - x) \tag{0.10}$$

Obs: even this eq. can be solved analytically.

A more complicated case: the Haber process. This process was developed by F. Haber in the early '900s for producing ammonia on an industrial scale: N_2(nitrogen)+$3H_2$(hydrogen) $\longrightarrow 2NH_3$ (ammonia) We consider then the reaction:

$$X + 3Y \underset{k_-}{\overset{k_+}{\rightleftarrows}} 2z \tag{0.11}$$

The ODEs for the concentrations are then:

$$\begin{cases} \dot{x} = -k_+ xy^3 + k_- z^2 \\ \dot{y} = -3k_+ xy^3 + 3k_- z^2 \\ \dot{z} = -2k_- z^2 + 2k_+ xy^3 \end{cases} \tag{0.12}$$

The stoichiometric coefficients enter the ODEs: Let's interpret the term $-3k_+ xy^3$ in eq. (11b)

Eq. (10) tells us that 3 molecules (or moles) of Y have to collide independently along with one molecule (or mole) of X for the reaction to occur in the forward (+) direction. Also, because for every molecule of X, three

molecules of Y react, for a decrease in concentration of x, there is a three fold decrease in concentration of Y. Thus, the stoichiometric coefficients affect the prob. of a reaction to occur as well as the relative speed of the reaction. Indeed, $3\dot{x} = \dot{y}$, which relates the two speeds of reaction. The term $3k_-z^2$ has a similar interpretation: for producing Y, two molecules (moles) of Z have to collide which will generate 3 molec. of Y. Also, for every 2 molec. of z that decompose in the backward direction (k_-), there will be 3 molec. of Y. This means that the speeds of reaction are $3|\dot{z}| = 2|\dot{y}|$. If we look at eq. 11.b,c we get $3\dot{z} = -2\dot{y}$ because the decrease of Y leads to an increase of z and vice versa.

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

$$3x(t) - y(t) = c_1, \quad 2x(t) + z(t) = c_2, \quad 2y(t) + 3z(t) = c_3 \tag{0.13}$$

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

More generally, we can restate the law of mass action as

0.1.4 The law of Mass Action

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

Ex: write down the rate equation for the reversible reaction in eq.(1)

$$2H_2 + O_2 \underset{k_-}{\overset{k_t}{\rightleftarrows}} 2H_2O \tag{0.14}$$

The general reaction

$$aX + bY \underset{k_-}{\overset{k_+}{\rightleftarrows}} cz + dW \quad a, b, c, d \in \mathbb{N} \tag{0.15}$$

leads to the following odes:

$$\begin{cases} \dot{x} = a\left(-k_+x^a y^b + k_-z^c w^d\right) \\ \dot{y} = b\left(-k_+x^a y^b + k_-z^c w^d\right) \\ \dot{z} = c\left(+k_+x^a y^b - k_-z^c w^d\right) \\ \dot{w} = d\left(+k_+x^a y^b - k_-z^c w^d\right) \end{cases} \tag{0.16}$$

Calculate the quantities that are conserved. There are types of molecules or species that can interact in different kinds of reactions: The predator

(Y) and prey (X) system: (irreversible reactions)

$$\begin{aligned} X &\xrightarrow{k_1} 2X \\ Y + X &\xrightarrow{k_2} 2Y \\ Y &\xrightarrow{k_3} \phi \end{aligned} \tag{0.17}$$

reproduction of preys, predator eats a prey, predator dies.

To get the ODEs we have simply to sum the effects of different reactions:

$$\begin{cases} \dot{x} = k_1 x - k_2 x y \\ \dot{y} = k_2 x y - k_3 y \end{cases} \tag{0.18}$$

These are the Lotka-Volterra equations. Show that at stationarity $\bar{x} = \frac{k_3}{k_2}, \bar{y} = \frac{k_1}{k_2}$ but the Jacobian at $(\bar{x}, \bar{y})$ has eigenvalues $\lambda = \pm i\sqrt{k_1 k_3}$. Is the system stable? Show that $V(x, y) = k_2(x + y) - k_3 \ln x - k_1 \ln y$ is a conserved quantity.

0.1.5 General chemical reactions

More generally we may consider m different chemical species $x_i, i = 1, 2 \dots m$ which are involved in n different reactions of the form

$$\sum_{i=1}^{m} a_{ij} X_i \underset{k_j^-}{\overset{k_j^+}{\rightleftarrows}} \sum_{i=1}^{m} b_{ij} X_i \quad j = 1, 2, \dots, n \tag{0.19}$$

where a_{ij} and b_{ij} are stoichiometric coefficients that are all non-negative integers.

Therefore the ODEs are

$$\dot{x}_i = \sum_{j=1}^{n} \left(b_{ij} - a_{ij}\right) r_j(\vec{x}) \quad i = 1, 2, \dots m \tag{0.20}$$

where $r_j(\bar{x}) \equiv k_j^+ \prod_{i=1}^{m} x_i^{a_{ij}} - k_j^- \prod_{i=1}^{m} x_i^{b_{ij}}$ for any $j = 1, 2, \dots, n$. We want to find the conservation laws of eq. (16). Let S be the stoichiometric matrix: $S_{ij} \equiv b_{ij} - a_{ij}$ This is a $m \times n$ matrix. In vector form eq. (16) reads

$$\frac{d}{dt}\vec{x} = S\vec{r}(\vec{x}) \tag{0.21}$$

A linear conserv. law for the system (15) or (16) has the form (if it exists)

$$\frac{d}{dt} \sum_{i=1}^{m} c_i x_i = 0 \tag{0.22}$$

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

$$\sum_i c_i x_i(t) = \sum_i c_i x_i(0) = \vec{c}^{\top} \cdot \vec{x}(0) \tag{0.23}$$

where $\vec{c}^\top = (c_1, c_2, \ldots, c_m)$. If we multiply eq eq (17) by $\vec{c}^\top$, then

$$\vec{c}^\top \cdot \frac{d}{dt}\vec{x} = \vec{c}^\top S\vec{r}(\vec{x}) = 0 \tag{0.24}$$

Eq. (19) holds true for all $\vec{r}$, hence it must be

$$\vec{c}^\top S = 0 \quad \text{or} \quad S^\top \vec{c} = 0 \tag{0.25}$$

The conservation laws of the system of reactions in eq - (16) are given by the non-zero elements $\vec{c} \in \ker(S^\top)$ ($\vec{c}^\top \cdot \vec{x} = \text{const}$) and the number of (linearly independent) conservation laws is given by $\dim(\ker(s^\top))$. For the reaction

Basis $(1, -1, 0)$ and $(1, 0, 1) \longrightarrow x - y = \text{const}$.

$$x + z = \text{ const.} \tag{0.26}$$

Tools for the simulation of chemical reactions Many tools and libraries are available for the numerical simulation of chemical reactions:

It is good practice to write down your own code for you to check whether you have understood the basics of the theory.

Also, these reactions should be implemented with stochastic algorithms which account for the discrete nature of the particles. These tools will be provided in the other part of the module.

Fokker-Planck equation **First Semester**

Lecture 2

Date: 2025-10-17 Profesor: Azaele Sandro

0.2 Fokker-Planck equation

Derivation of the Fokker-Planck equation for a general Langevin equation (Itô prescription)

We start from a stochastic process defined via the Langevin equation (Itô)

$$dx(t) = \mu(x(t), t)dt + \sigma(x(t), t)dB(t) \tag{0.27}$$

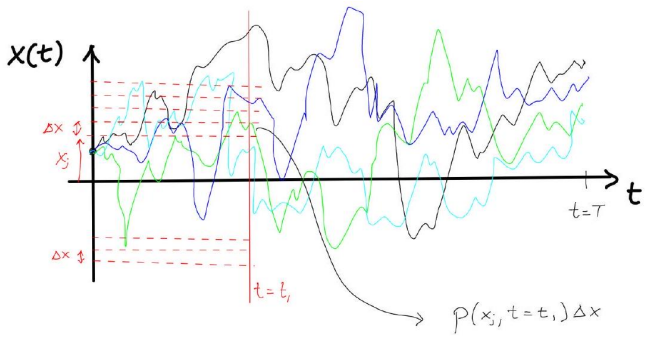
where $x(0) = x_0$ (or a generic initial PDF). $B(t)$ is a standard Brownian process. An alternative way to write eq. (1) is the "pseudo-equation"

$$\dot{x} = \mu(x, t) + \sigma(x, t)\xi(t) \tag{0.28}$$

Where $\langle \xi(t) \rangle = 0$ and $\langle \xi(t')\, \xi(t) \rangle = \delta(t' - t)$. We used the suggestive relation " $\frac{dB}{dt} = \xi$ ", even though this is only a formal, notational expression.

Eq. (1) defines the process $x(t)$ so we can use the eq. to generate as many trajectories as we wish. Let us assume that we have generated a large number N of paths from time $t = 0$ to $t = T > 0$. How can we calculate the probability that $x(t)$ gets a value between x and $x + \Delta x$ (a PDF) at time t?

From the computational point of view this is relatively easy:



We have to count how many paths fall in the interval $[x, x + \Delta x)$ at time $t = t_1$ as x varies in the domain of definition of the process $x(t)$. If we use the indicator function, I, defined as

$$I(a, A) = \begin{cases} 1 a \in A \\ 0 a \notin A \end{cases} \tag{0.29}$$

then we calculate numerically $P(x, t)$ as

$$P\left(x_j, t = t_1\right) \Delta x = \lim_{N \to \infty} \frac{1}{N} \sum_{1}^{N} I\left(x^i\left(t_1\right), \left[x_j, x_j + \Delta x\right)\right) \tag{0.30}$$

for any x_j and various t.

Where $x_j = j\Delta x$ and $j = j_{\min}, j_{\min} + 1, \ldots j_{\max} - 1, j_{\max}$ (uniform mesh). For example, if the process was Brownian, then $P(x, t)$ would be very well approximated by a Gaussian distribution with zero mean and variance t,

as we saw before. Notice that if we say $x_j = x, t = t$, and take the limit $\Delta x \to 0$, then

$$P(x,t) = \lim_{N\to\infty} \frac{1}{N}\sum_i^N \delta\left(x - x_i(t)\right) \text{ as } \lim_{\Delta x\to 0} \frac{I\left(x^i(t), [x, x+\Delta x)\right)}{\Delta x} = \delta\left(x - x_i(t)\right) \tag{0.31}$$

From the theoretical point of view we want to find out an equation for $P(x,t)$ which gives the PDF of the process $x(t)$. If we are interested in the statistics of the process, then $P(x,t)$ gives all the information we need, for we can calculate all averages we want (all moments) (even though it is not guaranteed that from the PDF we can exactly reconstruct the process $x(t)$ pathwise). Actually, we can calculate the average of any "sufficiently regular" function f. Let's assume that f has compact support in $\mathbb{R}$ and is twice-differentiable, namely $f \in C_c^2(\mathbb{R})$. Then we can calculate $\langle f(x(t))\rangle$, average of f over the process. If we are given N indep. realizations of $x(t)$, then as $N \to \infty$

$$\rangle = \lim_N \frac{1}{N}\sum_i^N f\left(x_i(t)\right) = \lim_N \frac{1}{N}\sum_i^N \int dx f(x)\delta\left(x - x_i(t)\right) = \int dx f(x) \lim_N \frac{1}{N}\sum_i^N \delta\left(x - x_i(t)\right) \overset{\downarrow}{=} \int dx f(x) p(x,t) \tag{0.32}$$

Hence

$$\frac{d}{dt}\langle f(x(t))\rangle \equiv \int \dot{p}(x,t) f(x) dx \tag{0.33}$$

Here $\langle \cdots \rangle$ means that the average of f has to be calculated over the whole set of trajectories of the process $x(t)$. We now discretize the process in time and Taylor-expand the function $f(x)$:

$$f(x(t+\Delta t)) = f(x(t)) + \Delta x f'(x(t)) + \frac{\Delta x^2}{2} f''(x(t)) + \text{ h.o.t.} \tag{0.34}$$

where from eq. (1) we get

$$\Delta x \equiv x(t+\Delta t) - x(t) = \mu(x(t),t)\Delta t + \sigma(x(t),t)\Delta B(t) \tag{0.35}$$

Therefore from (6) $\Delta f \equiv f(x(t+\Delta t)) - f(x(t))$

$$\begin{aligned} \Delta f &= f'(\mu\Delta t + \sigma\Delta B) + \frac{1}{2} f''(\mu\Delta t + \sigma\Delta B)^2 + \text{ h.o.t.} \\ &= f'(\mu\Delta t + \sigma\Delta B) + \frac{1}{2} f''\left(\mu^2\Delta t^2 + 2\mu\sigma\Delta t\Delta B + \sigma^2\Delta B^2\right) + \text{ h.o.t.} \end{aligned} \tag{0.36}$$

We now consider the average of each term: a) $\left\langle f'\sigma\Delta B\right\rangle = \left\langle f'\sigma\right\rangle\langle\Delta B\rangle = 0$ (Itô prescription) b) $\left\langle f''\mu\sigma\Delta t\Delta B\right\rangle = \left\langle f''\mu\sigma\right\rangle \Delta t\langle\Delta B\rangle = 0$ c) $\frac{1}{2}\left\langle f''\sigma^2\Delta B^2\right\rangle = \frac{1}{2}\left\langle f''\sigma^2\right\rangle\left\langle\Delta B^2\right\rangle = \frac{1}{2}\left\langle f''\sigma^2\right\rangle\Delta t$ (Itô preser. IMPORTANT!) all remaining terms are $O\left(\Delta t^2\right)$. Therefore eq. (5) can be re-written as limit

$$\lim_{\Delta t\to 0}\left\langle\frac{\Delta f}{\Delta t}\right\rangle = \left\langle f'\mu\right\rangle + \frac{1}{2}\left\langle f''\sigma^2\right\rangle = \int dx p(x,t)\left[f'(x)\mu(x,t) + \frac{1}{2}f''(x)\sigma^2(x,t)\right] \tag{0.37}$$

As $f \in C_c^2(\mathbb{R})$ we can integrate by parts and safely assume that f, f' and $f'' \to 0$ as $|x|$ is large enough. Hence

$$\int dx p(x,t)\mu(x,t)\frac{\partial f}{\partial x} \overset{\downarrow}{=} -\int dx f(x)\frac{\partial}{\partial x}(p\mu) \tag{0.38}$$

twice integrated by parts

$$\int dx p(x,t) \frac{\sigma^2(x,t)}{2} \frac{\partial^2 f}{\partial x^2} = \frac{1}{2} \int dx f(x) \frac{\partial^2}{\partial x^2} \left(\sigma^2(x) p\right) \tag{0.39}$$

and

$$\frac{d}{dt}\langle f(x)\rangle = \int dx f(x) \frac{\partial}{\partial t} p(x,t) \tag{0.40}$$

Thus from eqs. (9) and (10) and because $f \in C_c^2(\mathbb{R})$ but arbitrary we end up with

$$\frac{\partial}{\partial t} p(x,t) = -\frac{\partial}{\partial x}[\mu(x,t)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[\sigma^2(x,t)p(x,t)\right] \tag{0.41}$$

This is the forward Fokker-Planck equation corresponding to the process defined in eq. (1) with the Itô prescription. The FP eq. (11) can be used to derive the propagator of the process $x(t)$; we need just to solve it with the initial condition $P(x,t_0) = \delta(x - x_0)$, namely, this gives the fundamental solution $P(x,t \mid x_0,t_0)$. If we can calculate $P(x,t)$ then we can find all the averages (= statistics) of the process defined by the Langevin eq. (1). Notice that eq. (11) is a deterministic and linear PDE for $p(x,t)$.

Eq. (11) can also be written as

$$\frac{\partial p}{\partial t} = -\frac{\partial J}{\partial x}(x,t) \tag{0.42}$$

$$J(x,t) \equiv \mu(x,t)p(x,t) - \frac{1}{2}\frac{\partial}{\partial x}\sigma(x,t)p(x,t) \tag{0.43}$$

where $J(x,t)$ is the flux at x at time t. This form shows that, if the process $x(t)$ is defined in the domain $D \subseteq \mathbb{R}$, then

$$\frac{\partial}{\partial t}\int_D p(x,t)dx = -\int_D \frac{\partial J}{\partial x} dx = -J|_{x\in\partial D} \tag{0.44}$$

where ∂D is the boundary of D. If there is no "leakage" of probability, then $J|_{x\in\partial D} = 0$ and we can set $\int_D p(x,t)dx = 1$ at any time t (conservation of probability).

Notice that eq. (11) must be equipped with boundary conditions if the process $x(t)$ is defined in given domain $D \subset \mathbb{R}$. For instance, if $D = \mathbb{R}^+$one has to define what happens at $x = 0$ at any time $t > 0$.

* Absorbing boundary conditions require: $p(x,t)\big|_{x\in\partial D} = 0, \forall t$ * Reflecting boundary conditions require: $J(x,t)|_{x\in\partial D} = 0 \quad \forall t$ N.B: these are the correct conditions when $\sigma(x,t)|_{x\in\partial D} > 0 \quad \forall t$

Equilibrium solution of the Fokker-Planck equation

Let us assume that $\mu(x,t) = \mu(x)$ and $\sigma(x,t) = \sigma(x)$ and also that the propagator defined by eq. (11) reaches an equilibrium solution, namely

$$\lim_{t\to\infty} p(x,t \mid x_0,t_0) = p^{st}(x) \tag{0.45}$$

what is the form of $p^{st}(x)$? From. eq. (11) $\partial_t p^{st} = 0$ implies

$$-\frac{\partial}{\partial x}\left(\mu(x)p^{st} - \frac{1}{2}\frac{\partial}{\partial x}\sigma^2(x)p^{st}\right) = 0 \tag{0.46}$$

hence

$$J^{st}(x) = \mu(x)p^{st} - \frac{1}{2}\frac{\partial}{\partial x}\sigma^2(x)p^{st} = \text{ const for any } x\,. \tag{0.47}$$

If there is no current at any point $x \in D$, we obtain the equilibrium solution (with reflecting boundary conditions at ∂D)

$$\mu(x)p^{st}(x) = \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma^2(x)p^{st}(x)\right) \tag{0.48}$$

Since

$$\begin{aligned} &\frac{2\mu}{\sigma^2}\left(\sigma^2 p^{st}\right) = \frac{\partial}{\partial x}\left(\sigma^2 p^{st}\right) \\ &\sigma^2 p^{st} = \text{ const } e^{\int^x \frac{2\mu}{\sigma^2}dy} \end{aligned} \tag{0.49}$$

hence the equilibrium solution has the form (ref.bound. at x_m, x_M)

$$p^{st}(x) = \frac{1}{Z}\frac{1}{\sigma^2(x)}e^{2\int_{x_m}^x \frac{\mu(y)}{\sigma^2(y)}dy} \quad x_m \le x \le x_M \tag{0.50}$$

where $Z \equiv \int_{x_m}^{x_M} \frac{dx}{\sigma^2(x)}e^{2\int_{x_m}^x \frac{\mu(y)}{\sigma^2(y)}dy} < \infty$, and $\int_{x_m}^{x_M} p^{st}(x)dx = 1$. Some caveats: Notice that eq. (13) may not exist. Also we have not proved that it is unique, nor that it can be reached by some initial conditions. Eq. (13) is only the form one expects if indeed an equilibrium solution exists. Indeed, it does not depend on initial conditions and the equilibrium sol. is only determined by μ and σ (and the ref.b.c.), so it is an intrinsic property of the system which is not tuned by how we initially prepare the system.

The Ornstein-Uhlenbeck process

As a simple application of what we have studied we investigate the O.-U. process. From previous lectures we know that it is defined by the SDE

$$\begin{cases} dx = -\mu x dt + \sigma dB(t) & \text{or} \quad \dot{x} = -\mu x + \sigma\xi_t \\ x(0) = x_0 & (\langle\xi_t\rangle = 0, \langle\xi_t\xi_{t'}\rangle = \delta(t-t')) \end{cases} \tag{0.51}$$

Where μ, σ are positive constants and B is the B.m. From e. (11) we obtain the F.P. equation for the PDF:

$$\dot{p} = -\frac{\partial}{\partial x}[(-\mu x)p] + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}p \tag{0.52}$$

The equilibrium distribution of (15) (from eq. (13)) is

$$p^{st}(x) \propto e^{-\frac{2}{\sigma^2}\int^x \mu y dy} = e^{-\frac{\mu}{\sigma^2}x^2} \tag{0.53}$$

$$p^{st}(x) = \sqrt{\frac{\mu}{\pi\sigma^2}}e^{-\frac{\mu}{\sigma^2}x^2} \tag{0.54}$$

which is a Gaussian distribution with mean 0 and variance $\frac{\sigma^2}{2\mu}$. Exercise: Show that the equation for the variance that one gets from eq. (14) is the same that one gets from eq. (15). Verify that at stationarity the value is $\sigma^2/2\mu$.

Indeed one can calculate the evolution in time of the PDF.

By taking the Fourier transform of eq. (15) (which gives you the time evolution of the characteristic function of the process) one finds the full solution (which is the propagator of the O.-U. process)

$$p\left(x,t \mid x_0,s\right) = \sqrt{\frac{\mu}{\pi\sigma^2\left(1-e^{-\mu(t-s)}\right)}} e^{-\frac{\mu}{\sigma^2}\frac{\left(x-x_0e^{-\mu(t-s)}\right)^2}{1-e^{-\mu(t-s)}}} \tag{0.55}$$

for which $P\left(x,s \mid x_0,s\right) = \delta\left(x-x_0\right)$. Another way to find the solution is to start from the ansatz

$$p(x,t) \propto e^{-Ax^2+xB+C} \tag{0.56}$$

sub this into eq. (15) and find A, B and C as a function of t and x_0. The normalization and the initial condition finally give eq.(17).

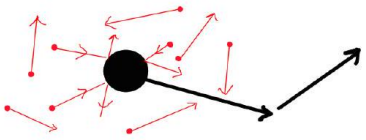
All these findings can be generalized to the case

$$\dot{p} = -\frac{\partial}{\partial x}[(\alpha-\mu x)p] + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}p \tag{0.57}$$

and also to the multidimensional O.-U. process (Gardiner, p. 105).

Particle in a large medium

We study the motion of a particle suspended in a large (fluid) medium. The particle should be much bigger than those of the medium but small enough to change position and momentum when colliding with the medium's particles. The surrounding medium is a heat bath at thermal equilibrium with a const. temperature T (homogeneous and isotropic). If we had to account for all interactions of the suspended (mesoscopic) particle of mass m, we would write



* Fluid particles at temp T * mesoscopic particle

$$m\ddot{\vec{x}}(t) = \vec{F}_{\text{ext}}\left(\vec{x}(t)\right) + \sum_i^N i\vec{F}\left(\vec{x}(t)-\vec{x}_i(t)\right) \tag{0.58}$$

where $\vec{F}_{\text{ext}}$ is an external force that may (or not) be described by a potential, where the i-th particle exerts on susp. particle a force $\bar{F}\left(\bar{x}-\overline{x_i}\right)$. As $N \simeq N_A$ (Avogadro number), it is pointless to integrate eq. (18). It's

more appropriate to treat the medium particles in an effective way, like an effective force acting on the susp. particle. Thus

$$\sum_{i}^{N} i\vec{F}\left(\vec{x}(t)-\vec{x}_i(t)\right) \simeq \vec{F}_{\text{aver}} + \vec{F}_{\text{noise}} \tag{0.59}$$

As the mesoscopic particle collides with the smaller fluid particles there is viscous damping generated by the collisions in the fluid. If the velocity of the particle isn't too large we can approximate $\vec{F}_{\text{aver}} = -\gamma\vec{v} = -\gamma\dot{\vec{x}}$, γ being the damping coefficient. From hydrodynamics, we can set $\gamma = 6\pi\eta R$, η being the viscosity and R the Brownian particle's radius. We also assume that all fluid particles have independent motions and every particle's movement is independent on different time intervals (if not too small).

Also, if there is a time interval τ (much smaller of time intervals of observation Δt) large enough that in any two successive time intervals τ the motions of the mesoscopic particle can be considered independent events, then we can effectively approximate $\vec{F}_{\text{noise}}$ as a stochastic process that is proportional to a Brownian motion. For simplicity, let's consider the 1-d case with no external forces. So from (18)

$$m\ddot{x} = -\gamma\dot{x} + \sigma\xi(t) \tag{0.60}$$

where $\langle\xi\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = \delta(t-t')$. Notice that this process is non-Markovian. Let's multiply both sides by x, then

$$mx\frac{d}{dt}\dot{x} = -\gamma x\dot{x} + \sigma x\xi_t \tag{0.61}$$

Since $\frac{d^2}{dt^2}x^2 = 2\left(\dot{x}^2 + x\ddot{x}\right)$, then

$$\frac{m}{2}\frac{d^2}{dt^2}\left(x^2\right) - m\dot{x}^2 = -\frac{\gamma}{2}\frac{d}{dt}\left(x^2\right) + \sigma x\xi_t \tag{0.62}$$

Take the average of both sides and use Itô prescription:

$$\frac{m}{2}\frac{d^2}{dt^2}\left\langle x^2\right\rangle - m\left\langle\dot{x}^2\right\rangle = -\frac{\gamma}{2}\frac{d}{dt}\left\langle x^2\right\rangle \tag{0.63}$$

Because of the equipartition theorem in classical mechanics

$$\frac{m}{2}\left\langle\dot{x}^2\right\rangle = \frac{1}{2}k_BT \tag{0.64}$$

k_B : Boltzmann's constant hence T: absolute temperature

$$m\frac{d^2}{dt^2}\left\langle x^2\right\rangle + \gamma\frac{d}{dt}\left\langle x^2\right\rangle = 2k_BT \tag{0.65}$$

Define $y(t) = \frac{d}{dt}\left\langle x^2\right\rangle$, then (19b) becomes

$$m\dot{y} + \gamma y = 2k_BT \tag{0.66}$$

Whose solution is $y(t) = ce^{-\frac{\gamma}{m}t} + \frac{2k_BT}{\gamma}$ and c is an arbitrary constant. In suspended particles $\frac{m}{\gamma} \simeq 10^{-8}$sec, which on temporal scales of

observation is a tiny time. Hence for $t \gg 10^{-8}$sec, $y \simeq \frac{2k_BT}{\gamma}$ and

$$\frac{d}{dt}\left\langle x^2\right\rangle \simeq \frac{2k_BT}{\gamma} \tag{0.67}$$

so

$$\left\langle x^2(t)\right\rangle - \left\langle x_0^2\right\rangle = \frac{2k_BT}{\gamma}t \text{ for } t \gg 10^{-8}\text{sec} \tag{0.68}$$

linear increase of the mean square deviation. This reminds us of the simple Brownian motion. Indeed, let's start from

$$\dot{x} = \sqrt{2D}\xi_t \text{ or } dx = \sqrt{2D}dB(t) \tag{0.69}$$

which leads to the diffusive equation

$$\frac{\partial}{\partial t}p(x,t) = D\frac{\partial^2}{\partial x^2}p(x,t) \quad D \text{ is diffusivity} \tag{0.70}$$

From (21) $x(t) = x_0 + \sqrt{2D}B(t)$ and

$$\left\langle x^2\right\rangle = \left\langle x_0^2 + 2x_0\sqrt{2D}B(t) + 2DB(t)^2\right\rangle = x_0^2 + 2Dt \tag{0.71}$$

diffusion law

By comparing eq. (20) and (22), we obtain

$$D = \frac{k_BT}{\gamma} \tag{0.72}$$

Einstein's relation

This is the first and simplest example of fluctuation-dissipation theorem.

Obs:

* Eq. (23) tells how we should choose the diffusivity if we want to interpret physically the mesoscopic particle as a free particle within an equilibrium thermal bath at temper. T. * D does not depend on initial conditions, or the nature of interactions between the fluid particles and the Brownian particle, all we need to know is that the system is at equilibrium in a system where general behavior is summarized by the damping constant γ. (We captured some universal behavior here!). * From the diffusion law in eq. (22) one can measure D, hence we can give an estimate of k_B and $N_A = \frac{R}{k_B}$, the Avogadro number (R is the gas constant). This is what Einstein suggested in his 1905 pioneering work on Brownian motion. * This interpretation is straightforward if we start from eq. (19) with $\sigma = \sqrt{2\gamma k_BT}$ and then take the limit $\frac{m}{\gamma} \to 0$ which is called the overdamped limit:

$$\frac{m}{\gamma}\ddot{x} = -\dot{x} + \frac{\sqrt{2\gamma k_BT}}{\gamma}\xi_t \xrightarrow{m/\gamma\to 0} \quad \dot{x} = \sqrt{2\frac{k_BT}{\gamma}}\xi_t \tag{0.73}$$

overdamped Langevin equation

Connection with Statistical Mechanics

From stat. Mech. we know how to calculate the PDF that a particle has momentum $\vec{p}$ and position $\vec{x}$ when it is located within an external potential $U(\vec{x})$ and is surrounded by a heat bath at equilibrium at temperature T. This is

$$\mathbb{P}(\vec{x},\vec{p}) = \frac{1}{z} e^{-\beta\left(\frac{\vec{p}^2}{2m}+U(\vec{x})\right)} \qquad \begin{array}{r}\text{Boltzmann's weight} \\ \beta = \dfrac{1}{k_B T}\end{array} \tag{0.74}$$

where m is the mass of the particle, $z = \int d\vec{p} \int d\vec{x}\mathbb{P}(\bar{x},\bar{p}) = (2\pi m k_B)^{3/2} z_0$ is the total partition function and z_0 the reduced one. From eq. (24) one gets the PDF to observe the particle at $\vec{x}$ at equilibrium regardless of its momentum. This is

$$w(\vec{x}) = \frac{1}{z_0} e^{-\beta U(\vec{x})} \tag{0.75}$$

Can we connect these classical results with the theory we have developed so far? Yes! We will do it for a 1-d system, but the generalization is simple and direct. Let's start from eq. (19) where now we assume that the particle experiences a conservative external force $f_{\text{ext}} = -\partial_x U(x)$, being $U(x)$ the potential of the force. We also assume that the Brownian particle is at equil. with the heat bath at temper. T, so $\sigma = \sqrt{2\gamma k_B T}$:

$$m\ddot{x} = -\partial_x U(x) - \gamma\dot{x} + \sqrt{2\gamma k_B T}\xi_t \tag{0.76}$$

In the overdamped limit ($\frac{m}{\gamma} \to 0$) we get

$$\dot{x} = -\frac{\partial_x U}{\gamma} + \sqrt{2D}\xi_t \quad D = \frac{k_B T}{\gamma} \tag{0.77}$$

or

$$dx = -\frac{1}{\gamma}\partial_x U dt + \sqrt{2D}dB(t) \tag{0.78}$$

The corresponding Fokker-Planck equation of eq. (27) is

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}\left[-\frac{1}{\gamma}\left(\partial_x U\right)p\right] + D\frac{\partial^2}{\partial x^2}p \tag{0.79}$$

You can check that the equilibrium distribution of eq. (28) is given by (see eq eq. (13))

$$P_{\text{eq}}(x) \propto e^{-\frac{1}{D\gamma}\int^x \partial_y U(y)dy} \propto e^{-\frac{1}{D\gamma}U(x)} \tag{0.80}$$

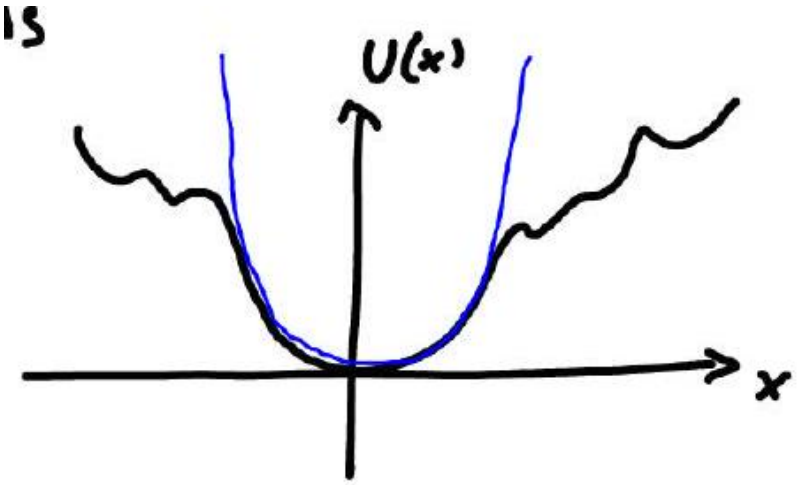
but $D\gamma = k_B T$, so $P_{\text{eq}}(x)$ and $w(x)$ in eq. (25) are exactly the same.

Obs:

* Notice that we could have fixed $D = \frac{k_B T}{\gamma}$ by imposing that eq eq. (29) and (25) are the same! This is remarkable and shows that the value of D does not depend on the potential U, which is somehow unexpected and

confirms the universality of Einstein's relation in eq. (23). * Notice that if $U(x) = \frac{1}{2}kx^2$, then eq. (27) reads

$$dx = -\frac{k}{\gamma}x dt + \sqrt{2\frac{k_B T}{\gamma}}dB(t) \tag{0.81}$$



which is an O.-U. process with the equilibrium distribution:

$$p_{\text{eq}}(x) = \sqrt{\frac{k\beta}{2\pi}}e^{-\frac{1}{2}\beta k x^2} \tag{0.82}$$

Brownian particle in contact with a heat bath at equilibrium and forced by a harmonic potential. We start from eq. (26) where $U(x) = \frac{1}{2}kx^2$ and $\sigma = \sqrt{2\gamma k_B T}$:

$$m\ddot{x} = -kx - \gamma\dot{x} + \sqrt{2\gamma k_B T}\xi_t \tag{0.83}$$

where x is the particle coordinate at time t, m its mass, γ the friction coefficient as before. Eq. (30) is a linear eq. and can be solved even though the process is non-Markovian because of $\ddot{x}$. We write

$$x(t) = x_c(t) + x_\xi(t) \tag{0.84}$$

where x_c satisfies the homogeneous eq.($\xi = 0$) with $x_c(0) = x_0$ and $\dot{x}_c = v_0$. x_ξ satisfies the in-homog. eq. with $x_\xi(0) = 0$ and $\dot{x}_\xi(0) = 0$. Show that

$$x_c(t) = Ae^{-\gamma_0 t}\sin(\Omega t) + Be^{-\gamma_0 t}\cos(\Omega t) \tag{0.85}$$

where A, B are arbitrary constants and

$$\gamma_0 = \frac{\gamma}{2m}, \quad \Omega = \omega_0^2 - \gamma_0^2, \quad \omega_0^2 = \frac{k}{m}; \tag{0.86}$$

and

$$x_\xi(t) = \sqrt{2\gamma k_B T}\frac{1}{m\Omega}\int_0^t e^{-\gamma_0(t-s)}\sinh[\Omega(t-s)]\xi(s)ds \tag{0.87}$$

Prove that

$$\left\langle x^2(t)\right\rangle = \frac{2\gamma k_B T}{m^2\Omega^2}\int_0^t e^{-2\gamma_0(t-s)}\sinh^2[\Omega(t-s)]ds \underset{t\to\infty}{\longrightarrow} \frac{k_B T}{m\omega_0^2} \quad (0.88)$$

* Can you interpret this result from the physical point of view? * Repeat the calculations for the velocity $v(t) = \dot{x}$ * Can you calculate $\langle x(t)x(s)\rangle$? If necessary, fix $|t-s|$ and take the limit $t \to \infty, s \to \infty$.

Fokker-Planck equation derivation **First Semester**

Lecture 3

Date: 2025-10-17 Profesor: Azaele Sandro

0.3 Fokker-Planck equation derivation

Derivation of the Fokker-Planck equation for a general Langevin equation (Itô prescription)

We start from a stochastic process defined via the Langevin equation (Itô)

$$dx(t) = \mu(x(t), t)dt + \sigma(x(t), t)dB(t) \tag{0.89}$$

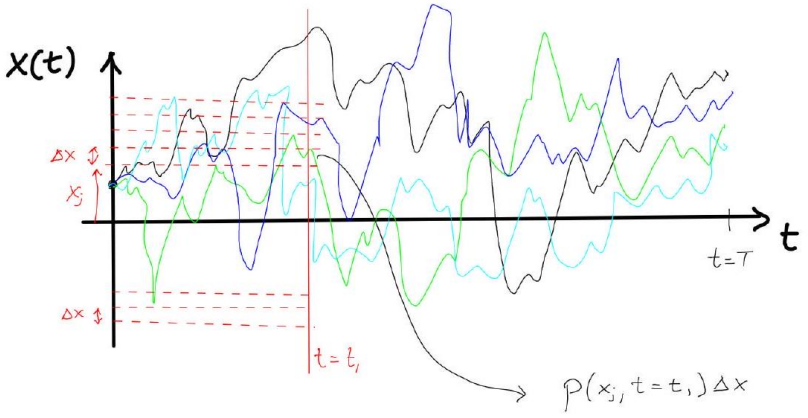
where $x(0) = x_0$ (or a generic initial PDF). $B(t)$ is a standard Brownian process. An alternative way to write eq. (1) is the "pseudo-equation"

$$\dot{x} = \mu(x, t) + \sigma(x, t)\xi(t) \tag{0.90}$$

Where $\langle \xi(t) \rangle = 0$ and $\langle \xi(t')\, \xi(t) \rangle = \delta(t' - t)$. We used the suggestive relation " $\frac{dB}{dt} = \xi$ ", even though this is only a formal, notational expression.

Eq. (1) defines the process $x(t)$ so we can use the eq. to generate as many trajectories as we wish. Let us assume that we have generated a large number N of paths from time $t = 0$ to $t = T > 0$. How can we calculate the probability that $x(t)$ gets a value between x and $x + \Delta x$ (a PDF) at time t?

From the computational point of view this is relatively easy:



We have to count how many paths fall in the interval $[x, x + \Delta x)$ at time $t = t_1$ as x varies in the domain of definition of the process $x(t)$. If we use the indicator function, I, defined as

$$I(a, A) = \begin{cases} 1 a \in A \\ 0 a \notin A \end{cases} \tag{0.91}$$

then we calculate numerically $P(x, t)$ as

$$P\left(x_j, t = t_1\right) \Delta x = \lim_{N \to \infty} \frac{1}{N} \sum_{1}^{N} I\left(x^i\left(t_1\right), \left[x_j, x_j + \Delta x\right)\right) \tag{0.92}$$

for any x_j and various t.

Where $x_j = j\Delta x$ and $j = j_{\min}, j_{\min}+1, \dots j_{\max}-1, j_{\max}$ (uniform mesh). For example, if the process was Brownian, then $P(x,t)$ would be very well approximated by a Gaussian distribution with zero mean and variance t, as we saw before. Notice that if we say $x_j = x, t = t$, and take the limit $\Delta x \to 0$, then

$$P(x,t) = \lim_{N\to\infty} \frac{1}{N}\sum_i^N \delta\left(x - x_i(t)\right) \text{ as } \lim_{\Delta x\to 0} \frac{I\left(x^i(t),[x,x+\Delta x)\right)}{\Delta x} = \delta\left(x - x_i(t)\right) \tag{0.93}$$

From the theoretical point of view we want to find out an equation for $P(x,t)$ which gives the PDF of the process $x(t)$. If we are interested in the statistics of the process, then $P(x,t)$ gives all the information we need, for we can calculate all averages we want (all moments) (even though it is not guaranteed that from the PDF we can exactly reconstruct the process $x(t)$ pathwise). Actually, we can calculate the average of any "sufficiently regular" function f. Let's assume that f has compact support in $\mathbb{R}$ and is twice-differentiable, namely $f \in C_c^2(\mathbb{R})$. Then we can calculate $\langle f(x(t))\rangle$, average of f over the process. If we are given N indep. realizations of $x(t)$, then as $N \to \infty$

$$\langle f(x(t))\rangle = \lim_N \frac{1}{N}\sum_i^N f\left(x_i(t)\right) = \lim_N \frac{1}{N}\sum_i^N \int dx f(x)\delta\left(x - x_i(t)\right) = \int dx f(x) \lim_N \frac{1}{N}\sum_i^N \delta\left(x - x_i(t)\right) \overset{\downarrow}{=} \int dx f(x) p(x,t) \tag{0.94}$$

Hence

$$\frac{d}{dt}\langle f(x(t))\rangle \equiv \int \dot{p}(x,t) f(x) dx \tag{0.95}$$

Here $\langle \cdots \rangle$ means that the average of f has to be calculated over the whole set of trajectories of the process $x(t)$. We now discretize the process in time and Taylor-expand the function $f(x)$:

$$f(x(t+\Delta t)) = f(x(t)) + \Delta x f'(x(t)) + \frac{\Delta x^2}{2} f''(x(t)) + \text{ h.o.t.} \tag{0.96}$$

where from eq. (1) we get

$$\Delta x \equiv x(t+\Delta t) - x(t) = \mu(x(t),t)\Delta t + \sigma(x(t),t)\Delta B(t) \tag{0.97}$$

Therefore from (6) $\Delta f \equiv f(x(t+\Delta t)) - f(x(t))$

$$\begin{aligned} \Delta f &= f'(\mu\Delta t + \sigma\Delta B) + \frac{1}{2} f''(\mu\Delta t + \sigma\Delta B)^2 + \text{ h.o.t.} \\ &= f'(\mu\Delta t + \sigma\Delta B) + \frac{1}{2} f''\left(\mu^2\Delta t^2 + 2\mu\sigma\Delta t\Delta B + \sigma^2\Delta B^2\right) + \text{ h.o.t.} \end{aligned} \tag{0.98}$$

We now consider the average of each term: a) $\left\langle f'\sigma\Delta B\right\rangle = \left\langle f'\sigma\right\rangle\langle\Delta B\rangle = 0$ (Itô prescription) b) $\left\langle f''\mu\sigma\Delta t\Delta B\right\rangle = \left\langle f''\mu\sigma\right\rangle\Delta t\langle\Delta B\rangle = 0$ c) $\frac{1}{2}\left\langle f''\sigma^2\Delta B^2\right\rangle = \frac{1}{2}\left\langle f''\sigma^2\right\rangle\left\langle\Delta B^2\right\rangle = \frac{1}{2}\left\langle f''\sigma^2\right\rangle\Delta t$ (Itô preser. IMPORTANT!) all remaining terms are $O\left(\Delta t^2\right)$. Therefore eq. (5) can be re-written as limit

$$\lim_{\Delta t\to 0}\left\langle\frac{\Delta f}{\Delta t}\right\rangle = \left\langle f'\mu\right\rangle + \frac{1}{2}\left\langle f''\sigma^2\right\rangle = \int dx p(x,t)\left[f'(x)\mu(x,t) + \frac{1}{2}f''(x)\sigma^2(x,t)\right] \tag{0.99}$$

As $f \in C_c^2(\mathbb{R})$ we can integrate by parts and safely assume that f, f' and

$f'' \to 0$ as $|x|$ is large enough. Hence

$$\int dx p(x,t)\mu(x,t)\frac{\partial f}{\partial x} \overset{\downarrow}{=} -\int dx f(x)\frac{\partial}{\partial x}(p\mu) \tag{0.100}$$

twice integrated by parts

$$\int dx p(x,t)\frac{\sigma^2(x,t)}{2}\frac{\partial^2 f}{\partial x^2} = \frac{1}{2}\int dx f(x)\frac{\partial^2}{\partial x^2}\left(\sigma^2(x)p\right) \tag{0.101}$$

and

$$\frac{d}{dt}\langle f(x)\rangle = \int dx f(x)\frac{\partial}{\partial t}p(x,t) \tag{0.102}$$

Thus from eqs. (9) and (10) and because $f \in C_c^2(\mathbb{R})$ but arbitrary we end up with

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}[\mu(x,t)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[\sigma^2(x,t)p(x,t)\right] \tag{0.103}$$

This is the forward Fokker-Planck equation corresponding to the process defined in eq. (1) with the Itô prescription. The FP eq. (11) can be used to derive the propagator of the process $x(t)$; we need just to solve it with the initial condition $P(x,t_0) = \delta(x - x_0)$, namely, this gives the fundamental solution $P(x,t \mid x_0,t_0)$. If we can calculate $P(x,t)$ then we can find all the averages (= statistics) of the process defined by the Langevin eq. (1). Notice that eq. (11) is a deterministic and linear PDE for $p(x,t)$.

Eq. (11) can also be written as

$$\frac{\partial p}{\partial t} = -\frac{\partial J}{\partial x}(x,t) \tag{0.104}$$

$$J(x,t) \equiv \mu(x,t)p(x,t) - \frac{1}{2}\frac{\partial}{\partial x}\sigma(x,t)p(x,t) \tag{0.105}$$

where $J(x,t)$ is the flux at x at time t. This form shows that, if the process $x(t)$ is defined in the domain $D \subseteq \mathbb{R}$, then

$$\frac{\partial}{\partial t}\int_D p(x,t)dx = -\int_D \frac{\partial J}{\partial x}dx = -J|_{x\in\partial D} \tag{0.106}$$

where ∂D is the boundary of D. If there is no "leakage" of probability, then $J|_{x\in\partial D} = 0$ and we can set $\int_D p(x,t)dx = 1$ at any time t (conservation of probability).

Notice that eq. (11) must be equipped with boundary conditions if the process $x(t)$ is defined in given domain $D \subset \mathbb{R}$. For instance, if $D = \mathbb{R}^+$one has to define what happens at $x = 0$ at any time $t > 0$.

- Absorbing boundary conditions require: $p(x,t)\big|_{x\in\partial D} = 0, \forall t$
- Reflecting boundary conditions require: $J(x,t)|_{x\in\partial D} = 0 \quad \forall t$ N.B: these are the correct conditions when $\sigma(x,t)|_{x\in\partial D} > 0 \quad \forall t$

Equilibrium solution of the Fokker-Planck equation

Let us assume that $\mu(x,t) = \mu(x)$ and $\sigma(x,t) = \sigma(x)$ and also that the propagator defined by eq. (11) reaches an equilibrium solution, namely

$$\lim_{t\to\infty} p\,(x,t \mid x_0,t_0) = p^{st}(x) \tag{0.107}$$

what is the form of $p^{st}(x)$? From. eq. (11) $\partial_t p^{st} = 0$ implies

$$-\frac{\partial}{\partial x}\left(\mu(x)p^{st} - \frac{1}{2}\frac{\partial}{\partial x}\sigma^2(x)p^{st}\right) = 0 \tag{0.108}$$

hence

$$J^{st}(x) = \mu(x)p^{st} - \frac{1}{2}\frac{\partial}{\partial x}\sigma^2(x)p^{st} = \text{ const for any } x\,. \tag{0.109}$$

If there is no current at any point $x \in D$, we obtain the equilibrium solution (with reflecting boundary conditions at ∂D)

$$\mu(x)p^{st}(x) = \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma^2(x)p^{st}(x)\right) \tag{0.110}$$

Since

$$\begin{aligned} &\frac{2\mu}{\sigma^2}\left(\sigma^2 p^{st}\right) = \frac{\partial}{\partial x}\left(\sigma^2 p^{st}\right) \\ &\sigma^2 p^{st} = \text{ const } e^{\int^x \frac{2\mu}{\sigma^2}dy} \end{aligned} \tag{0.111}$$

hence the equilibrium solution has the form (ref.bound. at x_m, x_M)

$$p^{st}(x) = \frac{1}{Z}\frac{1}{\sigma^2(x)}e^{2\int_{x_m}^x \frac{\mu(y)}{\sigma^2(y)}dy} \quad x_m \le x \le x_M \tag{0.112}$$

where $Z \equiv \int_{x_m}^{x_M} \frac{dx}{\sigma^2(x)} e^{2\int_{x_m}^x \frac{\mu(y)}{\sigma^2(y)}dy} < \infty$, and $\int_{x_m}^{x_M} p^{st}(x)dx = 1$. Some caveats: Notice that eq. (13) may not exist. Also we have not proved that it is unique, nor that it can be reached by some initial conditions. Eq. (13) is only the form one expects if indeed an equilibrium solution exists. Indeed, it does not depend on initial conditions and the equilibrium sol. is only determined by μ and σ (and the ref.b.c.), so it is an intrinsic property of the system which is not tuned by how we initially prepare the system.

The Ornstein-Uhlenbeck process

As a simple application of what we have studied we investigate the O-U process. From previous lectures we know that it is defined by the SDE

$$\begin{cases} dx = -\mu x dt + \sigma dB(t) & \text{or} \quad \dot{x} = -\mu x + \sigma\xi_t \\ x(0) = x_0 & (\langle\xi_t\rangle = 0, \langle\xi_t\xi_{t'}\rangle = \delta\,(t-t')) \end{cases} \tag{0.113}$$

Where μ, σ are positive constants and B is the B.m. From e. (11) we obtain the F.P. equation for the PDF:

$$\dot{p} = -\frac{\partial}{\partial x}[(-\mu x)p] + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}p \tag{0.114}$$

The equilibrium distribution of (15) (from eq. (13)) is

$$p^{st}(x) \propto e^{-\frac{2}{\sigma^2}\int^x \mu y dy} = e^{-\frac{\mu}{\sigma^2}x^2} \tag{0.115}$$

$$p^{st}(x) = \sqrt{\frac{\mu}{\pi\sigma^2}} e^{-\frac{\mu}{\sigma^2}x^2} \tag{0.116}$$

which is a Gaussian distribution with mean 0 and variance $\frac{\sigma^2}{2\mu}$. Exercise: Show that the equation for the variance that one gets from eq. (14) is the same that one gets from eq. (15). Verify that at stationarity the value is $\sigma^2/2\mu$.

Indeed one can calculate the evolution in time of the PDF.

By taking the Fourier transform of eq. (15) (which gives you the time evolution of the characteristic function of the process) one finds the full solution (which is the propagator of the O.-U. process)

$$p\left(x,t \mid x_0,s\right) = \sqrt{\frac{\mu}{\pi\sigma^2\left(1-e^{-\mu(t-s)}\right)}} e^{-\frac{\mu}{\sigma^2}\frac{\left(x-x_0e^{-\mu(t-s)}\right)^2}{1-e^{-\mu(t-s)}}} \tag{0.117}$$

for which $P\left(x,s \mid x_0,s\right) = \delta\left(x-x_0\right)$. Another way to find the solution is to start from the ansatz

$$p(x,t) \propto e^{-Ax^2+xB+C} \tag{0.118}$$

sub this into eq. (15) and find A, B and C as a function of t and x_0. The normalization and the initial condition finally give eq.(17).

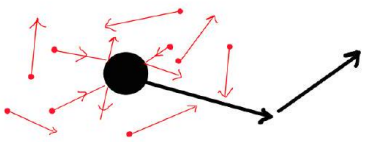
All these findings can be generalized to the case

$$\dot{p} = -\frac{\partial}{\partial x}[(\alpha-\mu x)p] + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}p \tag{0.119}$$

and also to the multidimensional O.-U. process (Gardiner, p. 105).

Particle in a large medium

We study the motion of a particle suspended in a large (fluid) medium. The particle should be much bigger than those of the medium but small enough to change position and momentum when colliding with the medium's particles. The surrounding medium is a heat bath at thermal equilibrium with a const. temperature T (homogeneous and isotropic). If we had to account for all interactions of the suspended (mesoscopic) particle of mass m, we would write



- Fluid particles at temp T
- mesoscopic particle

$$m\ddot{\vec{x}}(t) = \vec{F}_{\text{ext}}\left(\vec{x}(t)\right) + \sum_{i}^{N} i\vec{F}\left(\vec{x}(t) - \vec{x}_i(t)\right) \tag{0.120}$$

where $\vec{F}_{\text{ext}}$ is an external force that may (or not) be described by a potential, where the i-th particle exerts on susp. particle a force $\bar{F}\left(\bar{x} - \overline{x_i}\right)$. As $N \simeq N_A$ (Avogadro number), it is pointless to integrate eq. (18). It's more appropriate to treat the medium particles in an effective way, like an effective force acting on the susp. particle. Thus

$$\sum_{i}^{N} i\vec{F}\left(\vec{x}(t) - \vec{x}_i(t)\right) \simeq \vec{F}_{\text{aver}} + \vec{F}_{\text{noise}} \tag{0.121}$$

As the mesoscopic particle collides with the smaller fluid particles there is viscous damping generated by the collisions in the fluid. If the velocity of the particle isn't too large we can approximate $\vec{F}_{\text{aver}} = -\gamma\vec{v} = -\gamma\dot{\vec{x}}$, γ being the damping coefficient. From hydrodynamics, we can set $\gamma = 6\pi\eta R$, η being the viscosity and R the Brownian particle's radius. We also assume that all fluid particles have independent motions and every particle's movement is independent on different time intervals (if not too small).

Also, if there is a time interval τ (much smaller of time intervals of observation Δt) large enough that in any two successive time intervals τ the motions of the mesoscopic particle can be considered independent events, then we can effectively approximate $\vec{F}_{\text{noise}}$ as a stochastic process that is proportional to a Brownian motion. For simplicity, let's consider the 1-d case with no external forces. So from (18)

$$m\ddot{x} = -\gamma\dot{x} + \sigma\xi(t) \tag{0.122}$$

where $\langle\xi\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = \delta(t - t')$. Notice that this process is non-Markovian. Let's multiply both sides by x, then

$$mx\frac{d}{dt}\dot{x} = -\gamma x\dot{x} + \sigma x\xi_t \tag{0.123}$$

Since $\frac{d^2}{dt^2}x^2 = 2\left(\dot{x}^2 + x\ddot{x}\right)$, then

$$\frac{m}{2}\frac{d^2}{dt^2}\left(x^2\right) - m\dot{x}^2 = -\frac{\gamma}{2}\frac{d}{dt}\left(x^2\right) + \sigma x\xi_t \tag{0.124}$$

Take the average of both sides and use Itô prescription:

$$\frac{m}{2}\frac{d^2}{dt^2}\left\langle x^2\right\rangle - m\left\langle\dot{x}^2\right\rangle = -\frac{\gamma}{2}\frac{d}{dt}\left\langle x^2\right\rangle \tag{0.125}$$

Because of the equipartition theorem in classical mechanics

$$\frac{m}{2}\left\langle\dot{x}^2\right\rangle = \frac{1}{2}k_BT \tag{0.126}$$

k_B : Boltzmann's constant hence T: absolute temperature

$$m\frac{d^2}{dt^2}\left\langle x^2\right\rangle + \gamma\frac{d}{dt}\left\langle x^2\right\rangle = 2k_BT \tag{0.127}$$

Define $y(t) = \frac{d}{dt}\left\langle x^2 \right\rangle$, then (19b) becomes

$$m\dot{y} + \gamma y = 2k_B T \tag{0.128}$$

Whose solution is $y(t) = ce^{-\frac{\gamma}{m}t} + \frac{2k_B T}{\gamma}$ and c is an arbitrary constant. In suspended particles $\frac{m}{\gamma} \simeq 10^{-8}$sec, which on temporal scales of observation is a tiny time. Hence for $t \gg 10^{-8}$sec, $y \simeq \frac{2k_B T}{\gamma}$ and

$$\frac{d}{dt}\left\langle x^2 \right\rangle \simeq \frac{2k_B T}{\gamma} \tag{0.129}$$

so

$$\left\langle x^2(t) \right\rangle - \left\langle x_0^2 \right\rangle = \frac{2k_B T}{\gamma} t \text{ for } t \gg 10^{-8}\text{sec} \tag{0.130}$$

linear increase of the mean square deviation. This reminds us of the simple Brownian motion. Indeed, let's start from

$$\dot{x} = \sqrt{2D}\xi_t \text{ or } dx = \sqrt{2D}dB(t) \tag{0.131}$$

which leads to the diffusive equation

$$\frac{\partial}{\partial t}p(x,t) = D\frac{\partial^2}{\partial x^2}p(x,t) \quad D \text{ is diffusivity} \tag{0.132}$$

From (21) $x(t) = x_0 + \sqrt{2D}B(t)$ and

$$\left\langle x^2 \right\rangle = \left\langle x_0^2 + 2x_0\sqrt{2D}B(t) + 2DB(t)^2 \right\rangle = x_0^2 + 2Dt \tag{0.133}$$

diffusion law

By comparing eq. (20) and (22), we obtain

$$D = \frac{k_B T}{\gamma} \tag{0.134}$$

Einstein's relation

This is the first and simplest example of fluctuation-dissipation theorem.

Obs:

1. Eq. (23) tells how we should choose the diffusivity if we want to interpret physically the mesoscopic particle as a free particle within an equilibrium thermal bath at temper. T.
2. D does not depend on initial conditions, or the nature of interactions between the fluid particles and the Brownian particle, all we need to know is that the system is at equilibrium in a system where general behavior is summarized by the damping constant γ. (We captured some universal behavior here!).
3. From the diffusion law in eq. (22) one can measure D, hence we can give an estimate of k_B and $N_A = \frac{R}{k_B}$, the Avogadro number (R is the gas constant). This is what Einstein suggested in his 1905 pioneering work on Brownian motion.

4. This interpretation is straightforward if we start from eq. (19) with $\sigma = \sqrt{2\gamma k_B T}$ and then take the limit $\frac{m}{\gamma} \to 0$ which is called the overdamped limit:

$$\frac{m}{\gamma}\ddot{x} = -\dot{x} + \frac{\sqrt{2\gamma k_B T}}{\gamma}\xi_t \xrightarrow{m/\gamma \to 0} \quad \dot{x} = \sqrt{2\frac{k_B T}{\gamma}}\xi_t \tag{0.135}$$

overdamped Langevin equation

Turing Pattern Formation **First Semester**

Lecture 4

Date: 2025-10-17 Profesor: Azaele Sandro

0.4 Turing Pattern Formation

Nature offers a wide range of examples of biological patterns, from animal pigmentation to shells, skin, wings and skeletal structures. Patterns are composed of spatially heterogeneous structures which may emerge owing to several (biological) reasons. These could arise in systems in which chemicals react with each other and also underwent diffusion - a mechanism which is termed diffusion-driven instability. This is the basis of the so called Turing patterns.

Turing patterns and instability are related to symmetry breaking in non-equilibrium systems and represent an example of emergent pattern, namely, a structure that emerges from the combination of processes, which per se do not possess any property related to the pattern itself.

In 1952 Alan Turing (logician, computer scientist, code breaker and mathematician) proposed a mathematical model which was able to show emergent patterns (A.M. Turing, the chemical basis of morphogenesis, Philos. Trans. R. Soc. London B 237, 37-72, (1952)).

Turing showed that when some chemicals react with each other and diffuse appropriately, then spatially heterogeneous patterns can emerge (diffusion-driven instability), if some conditions are met.

One chemical species

Let us consider the case with one chemical species, diffusing in a one-dimensional space. We could consider the reactions

$$3U \underset{k_-}{\overset{k_+}{\rightleftarrows}} 2U \;\; \phi \quad \underset{\mu_-}{\overset{\mu_+}{\rightleftarrows}} U \Bigg\} \rightarrow \dot{u} = -k_+ u^3 + k_- u^2 - \mu_- u + \mu_{+1} \quad (0.136)$$

which involve only the species U (u is its concentration). For the sake of generality, let's assume that the chemical U is being produced at rate

$f(u)$ (typically a polynomial or a rational function of u). If we include diffusion

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} + f(u) \tag{0.137}$$

Where $D > 0$ is the diffusion coefficient. Eq. (1) is a reaction-diffusion equation. We also assume that U diffuses in a domain $(0, L)$ and that

$$u(0,t) = u_0 = u(L,t) \quad \forall t \tag{0.138}$$

These are called Dirichlet boundary conditions. If there is a spatially uniform stationary state u_0 for u, then we also have $\lim_{t\to\infty} u(x,t) = u_0$ and $f(u_0) = 0$. Is this state stable? In general this is a hard question, but we can check whether u_0 is linearly stable. To check this we have to determine the effect of a small perturbation. $\hat{u}(x,t) = u(x,t) - u_0 \quad (|\hat{u}| \ll u_0)$. Expanding f in a Taylor series we get (only linear terms) from eq. (1)

$$\frac{\partial \hat{u}}{\partial t} = D\frac{\partial^2 \hat{u}}{\partial x^2} + f'(u_0)\,\hat{u} \quad \hat{u}(0,t) = 0 = \hat{u}(L,t) \tag{0.139}$$

where we assumed $f(u_0) = 0$ and $f'(u_0) \neq 0$. Without space ($D = 0$) we get

$$\hat{u}(x,t) = \hat{u}_0 e^{f'(u_0)t} \tag{0.140}$$

$\hat{u}_0$ is the initial perturbation. Of course, the steady state is stable if $f'(u_0) < 0$. If $D > 0$, then eq. (3) can be solved via separation of variables: $\hat{u}(x,t) = h(x)k(t)$. Thus we get from eq. (3)

$$(\partial_t k)\,h = Dk\left(\partial_x^2 h\right) + f'(u_0)\,kh \quad \frac{\partial_t k}{k} = D\frac{\partial_x^2 h}{h} + f'(u_0) \tag{0.141}$$

because the l.h.s. depends on t only and the r.h.s. on x only, it must be

$$\underbrace{\frac{\partial_t k}{k}}_{a} = \lambda = \overbrace{D\frac{\partial_x^2 h}{h} + f'(u_0)}^{b} \tag{0.142}$$

Where λ is constant independent of time and space a) $\partial_t k = \lambda k \Rightarrow k(t) = k_0 e^{\lambda t}$ b) $\partial_{xx}^2 h = \underbrace{\frac{\lambda - f'(u_0)}{D}}_{-\rho^2} h \Rightarrow h(x) = A\sin(\rho x) + B\cos(\rho x)$

From the B.C. in eq. (2) we obtain $h(0) = 0 \Rightarrow B = 0$ and also $h(L) = 0 \Rightarrow \rho = \frac{n\pi}{L}$ for any $n = 1, 2\ldots$ Hence the modes

$$\lambda_n = f'(u_0) - D\left(\frac{n\pi}{L}\right)^2 \quad n = 1, 2, \cdots \tag{0.143}$$

Because the eq. is linear, we can sum all the modes and get the final solution as a Fourier series:

$$\hat{u}(x,t) = \sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{L}\right) e^{\lambda_n t} \quad \hat{u}(0,t) = 0 = \hat{u}(L,t) \tag{0.144}$$

where a_n are determined to satisfy the initial condition for the pert. Note from (5) that, even if $f'(u_0) > 0$ (u_0 is unstable), then $D > f'(u_0)\left(\frac{L}{\pi}\right)^2$ (for fixed domain size L) implies $\lambda_n < 0$. Therefore, all terms in eq. (6) with $a_n \neq 0$ have an expon. decay, hence $\hat{u} \to 0$ as $t \to \infty$. In this case the state u_0 is stabilized by diffusion, even when it is unstable, if D is sufficiently large. D cannot destabilize the solution.

0.4.1 Exercise:

If B.C. are zero-flux at the boundaries $\left(\frac{\partial u}{\partial x}(0) = 0 = \frac{\partial u}{\partial x}(L)\right.$, Neumann B.C.) the zeroth mode could still grow, but all the others decay exponentially so there cannot be any spatial heterogeneity for large D. Same arguments still hold for periodic B.C.

Obs: Notice that diffusivity is not always able to stabilize. If we fix D and increase L when $f'(u_0) > 0$, then for sufficiently large domain sizes $\left(L > \sqrt{\frac{D\pi^2}{f'(u_0)}}\right)$ we still get $\lambda_n > 0$. The effect of diffusion depends on the domain.

0.4.2 Two or more chemical species

From the previous section we have learnt that diffusion is able to smooth out inhomogeneities, thus stabilizing processes. This agrees with other phenomena, e.g., diffusion of heat within a finite domain. Turing understood that if there are more than one interacting species, this is not necessarily the case and diffusion may destabilize homogeneous solutions. Let $u(x,t)$ and $v(x,t)$ be the concentrations of two chemical species which satisfy the following reaction-diffusion equations in 1-d space:

$$\left.\begin{aligned} \dot{u} &= f(u,v) + D_1 \frac{\partial^2 u}{\partial x^2} \\ \dot{v} &= g(u,v) + D_2 \frac{\partial^2 v}{\partial x^2} \end{aligned}\right\} \quad \text{with I.C. and B.C.} \tag{0.145}$$

where f and g are smooth functions which describe the reactions between the two chemicals whose concentrations are given by u and v. D_1 and D_2 are two diffusion constants. We assume that $x \in (0, L)$ (finite domain) and at the boundaries we impose zero-flux conditions (Neumann b.c.).

Let us assume that eq. (7) admits a spatially uniform steady state, hence there exist u_0 and v_0 such that $f(u_0, v_0) = 0 = g(u_0, v_0)$. We now wish to derive conditions of linear stability for the state (u_0, v_0). For this we introduce small (spatially-dependent) perturbations $\hat{u}(x,t) = u(x,t) - u_0$ and $\hat{v}(x,t) = v(x,t) - v_0$ into eq. (7) and expand f and g in Taylor series. We arrive at (recall that $f(u_0, v_0) = 0, g(u_0, v_0) = 0$)

$$\left.\begin{aligned} \dot{\hat{u}} &= \left.\frac{\partial f}{\partial u}\right|_0 \hat{u} + \left.\frac{\partial f}{\partial v}\right|_0 \hat{v} + D_1 \frac{\partial^2 \hat{u}}{\partial x^2} \\ \dot{\hat{v}} &= \left.\frac{\partial g}{\partial u}\right|_0 \hat{u} + \left.\frac{\partial g}{\partial v}\right|_0 \hat{v} + D_2 \frac{\partial^2 \hat{v}}{\partial x^2} \end{aligned}\right. \tag{0.146}$$

where $\left.\frac{\partial f}{\partial u}\right|_0 \equiv \left.\frac{\partial f(u,v)}{\partial u}\right|_{u=u_0\ v=v_0}$ and the same for the rest. We can recast eq.

(8) in the matrix form

$$\begin{pmatrix}\partial_t \hat{u}\\ \partial_t \hat{v}\end{pmatrix} = \underbrace{\begin{pmatrix}\left.\frac{\partial f}{\partial u}\right|_0 & \left.\frac{\partial f}{\partial v}\right|_0 \\ \left.\frac{\partial g}{\partial u}\right|_0 & \left.\frac{\partial g}{\partial v}\right|_0\end{pmatrix}}_{\equiv J_0}\begin{pmatrix}\hat{u}\\ \hat{v}\end{pmatrix} + \underbrace{\begin{pmatrix}D_1 & 0\\ 0 & D_2\end{pmatrix}}_{\equiv D}\begin{pmatrix}\partial_x^2 \hat{u}\\ \partial_x^2 \hat{v}\end{pmatrix} \tag{0.147}$$

or

$$\frac{\partial}{\partial t}\overrightarrow{\hat{u}} = J_0 \overrightarrow{\hat{u}} + D\partial_x^2 \overrightarrow{\hat{u}} \tag{0.148}$$

We carry out the analysis of the previous section and look for a solution of the form

$$\vec{u}(x,t) = \vec{a} e^{\left(ikx + \lambda\left(k^2\right)t\right)} \tag{0.149}$$

where $\vec{a}$ is a constant vector. Subbing (10) into (9) we get

$$\lambda \vec{a} e^{ikx+\lambda t} = J_0 \vec{a} e^{ikx+\lambda t} - k^2 D \vec{a} e^{ikx+\lambda t} \tag{0.150}$$

which leads to the matrix equation

$$\left(J_0 - k^2 D - \lambda \mathbb{1}\right)\vec{a} = \overrightarrow{0} \tag{0.151}$$

where $\mathbb{1}$ is the unit 2×2 matrix and $\overrightarrow{0} = (0,0)^T$.

For non-trivial solutions to exist, we thus require that

$$\det\left(J_0 - k^2 D - \lambda \mathbb{1}\right) = 0 \tag{0.152}$$

this condition provides us equations for obtaining the eigenvalues λ (or temporal growth rates) which are functions of k^2. If we find $\mathrm{Re}\,\lambda > 0$ for at least one eigenvalue then the solution is unstable.

In the previous section we showed that an unstable fixed point can be stabilized. Here we show that a stable homogeneous fixed point can be destabilized by diffusion: this is the core of Turing pattern formation (and the Turing's brilliant idea). (1) A spatially-uniform steady state is linearly stable

Let us consider the case with no diffusion $D_1 = D_2 = 0$. Then λ is the eigenvalue of the matrix J_0:

$$\det\left(J_0 - \lambda\mathbb{1}\right) = \det\begin{pmatrix}\partial_u f - \lambda & \partial_v f\\ \partial_u g & \partial_v g - \lambda\end{pmatrix} = \left(\partial_u f - \lambda\right)\left(\partial_v g - \lambda\right) - \partial_u g \partial_v f = 0 \tag{0.153}$$

or

$$\lambda^2 - \underbrace{\left(\partial_u f + \partial_v g\right)}_{sum of sols}\lambda + \underbrace{\partial_u f \partial_v g - \partial_v f \partial_u g}_{prod. of sols.} = 0 \tag{0.154}$$

For the partially uniform steady state to be stable, both eigenvalues must have negative real part, this leads to require that

$$\partial_u f + \partial_v g < 0 \quad \mathrm{Tr}\left(J_0\right) < 0 \tag{0.155}$$

$$\partial_u f \partial_v g - \partial_v f \partial_u g > 0 \quad \mathrm{Det}\left(J_0\right) > 0 \tag{0.156}$$

(2) A spatially-uniform steady state is linearly stable and is destabilized

by diffusion

When D_1 and D_2 are not zero, diffusion plays a role and changes the eigenvalue problem. The determinant of eq. (12) leads to the equation

$$\lambda^2 - b\left(k^2\right)\lambda + c\left(k^2\right) = 0 \tag{0.157}$$

where

$$b\left(k^2\right) = \partial_u f + \partial_v g - \left(D_1 + D_2\right)k^2 \qquad c\left(k^2\right) = D_1 D_2 k^4 - \left(D_2\partial_u f + D_1\partial_v g\right)k^2 + \det\left(J_0\right) \tag{0.158}$$

For diffusion to destabilize the fixed point a necessary condition is that at least one of the roots of $\lambda\left(k^2\right)$ in eq. (16) has positive real part for some non-zero (positive) k^2. This can happen if either $b > 0$ or $c < 0$. Now

$$b = \partial_u f + \partial_v g \underbrace{- \left(D_1 + D_2\right)k^2}_{\leqslant 0} \leqslant \partial_u f + \partial_v g < 0 \quad \text{(from (14))} \tag{0.159}$$

So we must require $c\left(k^2\right) < 0$. Now because $\det(J_0) > 0$ (from (15)), we must necessarily have

$$D_2\partial_u f + D_1\partial_v g > 0 \tag{0.160}$$

Actually, this is a necessary, but not sufficient, condition for $\mathrm{Re}\,\lambda > 0$. For $c\left(k^2\right)$ to be negative for some $k \neq 0$, the minimum of c must be negative. The minimum of c is (check this!)

$$C_{\min} = \det J_0 - \frac{\left(D_2\partial_u f + D_1\partial_v g\right)^2}{4D_1 D_2} \tag{0.161}$$

which is obtained when k^2 is

$$k^2_{\min} = \frac{D_2\partial_u f + D_1\partial_v g}{2D_1 D_2} \tag{0.162}$$

Thus the condition $c\left(k^2\right) < 0$ requires $c_{\min} < 0$. From (18)

$$\frac{\left(D_2\partial_u f + D_1\partial_v g\right)^2}{4D_1 D_2} > \det J_0 \tag{0.163}$$

which gives (= indicates a critical (bifurcation) value)

$$D_2\partial_u f + D_1\partial_v g \geqslant 2\sqrt{D_1 D_2 \det J_0} > 0 \tag{0.164}$$

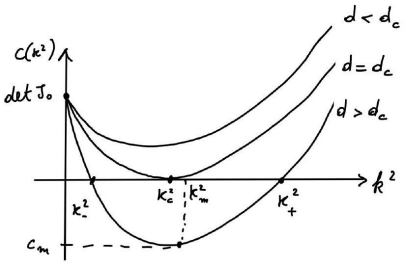


Figure 2: critical diffusivities ratio for Turing patterns to emerge.

Critical ratio (d_c)

At the bifurcation $C_{\min} = 0$, which can be obtained only when D_1 and D_2 have a specific ratio. From eq. (20) and $\frac{D_2}{D_1} = d$ we get

$$\left(d\partial_u f + \partial_v g\right)^2 \geqslant 4d \det J_0 > 0 \tag{0.165}$$

So the critical ratio d_c of diffusivities satisfies the equation

$$d_c^2 \left(\partial_u f\right)^2 + \left(\partial_v g\right)^2 + 2d\partial_u f \partial_v g - 4d \left(\partial_u f \partial_v g - \partial_v f \partial_u g\right) = 0 \tag{0.166}$$

or

$$d_c^2 \left(\partial_u f\right)^2 + 2\left(2\partial_v f \partial_u g - \partial_u f \partial_v g\right) d_c + \left(\partial_v g\right)^2 = 0 \tag{0.167}$$

From d_c we can calculate the critical wavenumber k_c^2. Indeed from eq eq eq. (19)

$$k_{\min}^2 = \frac{D_2\partial_u f + D_1\partial_v g}{2D_1D_2} = \frac{1}{D_1}\frac{d\partial_u f + \partial_v g}{2d} = \frac{1}{D_1}\sqrt{\frac{\det\left(J_0\right)}{d}} \tag{0.168}$$

from eq. (18) with $c_{\min} = 0$ from which we obtain (when $c_{\min} = 0$, $k_{\min} = k_c$):

$$k_c^2 = \frac{1}{D_1}\sqrt{\frac{\det\left(J_0\right)}{d_c}} \tag{0.169}$$

where d_c is from (21).

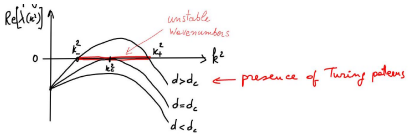
Conditions for Turing patterns to emerge

Conditions (14), (15) and (20) ensure that the spatially uniform state is linearly stable but has at least one wave number k for which $\lambda\left(k^2\right)$ has positive real part. When we impose zero-flux boundary conditions, wavenumbers are restricted to $k = \frac{n\pi}{L}$. Therefore there must exist at least one integer value $n = 1, 2 \ldots$ for which $c\left(k^2\right) < 0$ (in this case $d > d_c$). In this case the range of unstable wavenumbers is obtained from the zeros $k_\pm^2$ of $c\left(k^2\right) = 0$ (see eq. (17)). We get

$$k_\pm^2 = \frac{D_2\partial_u f + D_1\partial_v g \pm \sqrt{\left(D_2\partial_u f + D_1\partial_v g\right)^2 - 4D_1D_2\left(\partial_u f\partial_v g - \partial_v f\partial_u g\right)}}{2D_1D_2} \tag{0.170}$$

$$k_-^2 \leqslant \left(\frac{n\pi}{L}\right)^2 \leqslant k_+^2 \tag{0.171}$$

see also the previous figure and this one

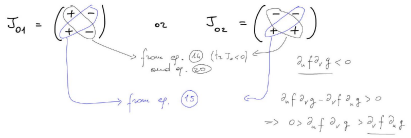


Important comments:

1. Because $\partial_u f + \partial_v g < 0$ (eq. (14)) and $D_2\partial_u f + D_1\partial_v g > 0$ (eq. (20)), it follows that $\partial_u f$ and $\partial_v g$ must be of opposite sign. If we take $\partial_u f > 0$ (activator) and $\partial_v g < 0$ (inhibitor) we get $\partial_u f < \left|\partial_v g\right|$. From eq. (20) we have $D_2\partial_u f + D_1\partial_v g > 0$, thus

$$\frac{D_2}{D_1} > -\frac{\partial_v g}{\partial_u f} = \frac{\left|\partial_v g\right|}{\partial_u f} > 1 \Rightarrow D_2 > D_1 \tag{0.172}$$

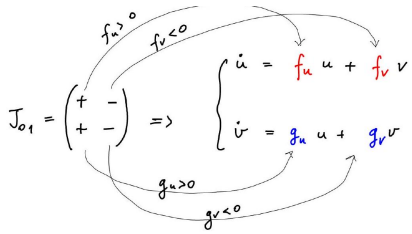
   This is usually summarized by saying that The inhibitor must diffuse faster than the activator.
2. From eq. (14) ($\mathrm{Tr}\,(J_0) < 0$), (15) ($\det J_0 > 0$) and eq. (20), it follows that J_0 must take one of the two forms: (u activ., v inhib.)

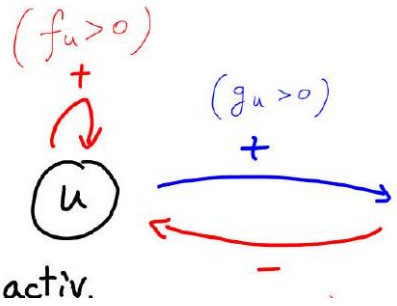


   on the alternative ones (v activ., u inhib.)

$$J_{03} = -J_{01} = \begin{pmatrix} - & + \\ - & + \end{pmatrix} \quad J_{04} = -J_{02} = \begin{pmatrix} + & + \\ - & - \end{pmatrix} \tag{0.173}$$

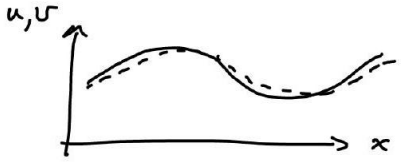
   for allowing the emergence of a Turing pattern.
3. When the linearized equations (see eq. (8)) at (u_0, v_0) have J_0 of the form J_{01}, we say that the system is a pure activator-inhibitor system. From eq. (8) and J_{01}



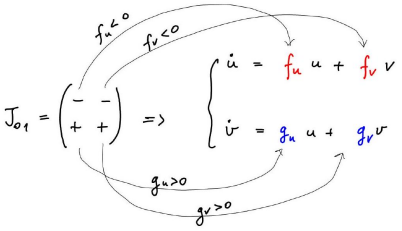


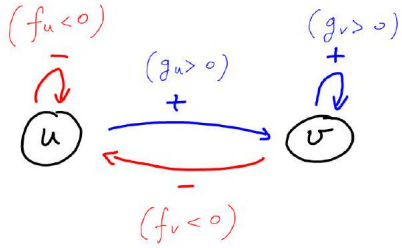
   (a) At steady state u activates its own production, but v inhibits the production of u; (b) At steady state u also activates the production of v, but v inhibits its own production.
   The equations and diagram show why u is termed ACTIVATOR, while v is termed INHIBITOR. Because we also have $D_2 > D_1$ we get short-range activation and long-range inhibition.

In this case u and v grow in phase: (look at the eigenvectors of J_{01})

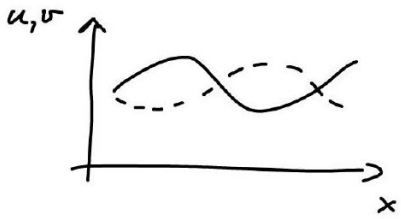


In the second case for J_{02}:





(c) At steady state, u inhibits its own production as well as v inhibits the production of u; (d) At steady state, u produces v, and v activates itself.
In this case the system is called cross-activator-inhibitor system and u and v grow out of phase (180°)



4. From eq. (23) it follows that there exists a minimum domain size for pattern formation. Indeed, for L sufficiently small, the inequality in (23) cannot be satisfied for $n > 0$.
5. As the domain size increases (L becomes larger), the number of viable integers also increases and the pattern will become more complicated.
6. Considerations in (3) and (4) can be extended to higher dimensions, where there may occur degeneracy. In $d = 2$

$$k^2 = \left(\frac{n\pi}{L_x}\right)^2 + \left(\frac{m\pi}{L_y}\right)^2 \quad n, m \in \mathbb{N} \tag{0.174}$$

Because there may exist multiple pairs (n, m) which produce the same k^2, in higher dimensions different patterns (say, stripes,

checkerboard, spots..) may emerge due to different initial conditions, which may combine different solutions (on the basis of the non-linear terms).

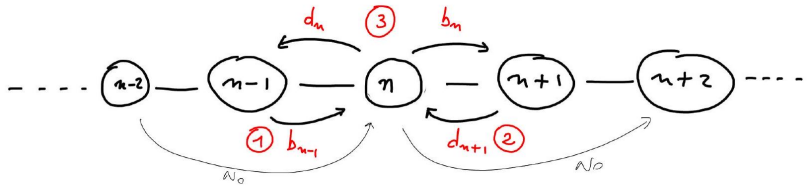
Birth and death Markov processes **First Semester**

Lecture 5

Date: 2025-10-17 Profesor: Azaele Sandro

0.5 Birth and death Markov processes

We discuss here a simple class of Markov processes, those that have a set of states that can be labeled with integers. We start from an even simpler discrete Markov process, the birth and death processes which occur in many applications. Then we will deduce results to more general cases. We start from a situation that is very similar to the random walk. We assume discrete times $t = 0, \Delta t, 2\Delta t, \ldots$ discrete states $x = 0, \pm 1, \pm 2 \ldots$ and that jumps are allowed only between nearest neighbors, i.e. from n to $n \pm 1$. For $\Delta t \ll 1$ we call $b_n \geqslant 0$ the birth rate, i.e., $b_n \Delta t$ is the prob. to jump to $n+1$ at time $t + \Delta t$, given that at time t the state was n. (notice that b_n does not depend on time, though it could in principle. If it does not, we say that the process is homogeneous). Analogously, $d_n \geqslant 0$ is the death rate, i.e. $d_n \Delta t$ is the prob. to jump to $n-1$ at time $t + \Delta t$, given that at time t the state was n. We want to calculate the prob. $p(n, t + \Delta t)$ (the propagator).



$$p(n, t + \Delta t) = b_{n-1}\Delta t\, p(n-1, t) + d_{n+1}\Delta t\, p(n+1, t) + [1 - (b_n + d_n)\Delta t]\, p(n, t) \tag{0.175}$$

By Taylor expansions and then taking the limit $\Delta t \to 0$ we get

$$\frac{\partial p_n}{\partial t} = b_{n-1} p_{n-1}(t) + d_{n+1} p_{n+1}(t) - (b_n + d_n)\, p_n(t) \tag{0.176}$$

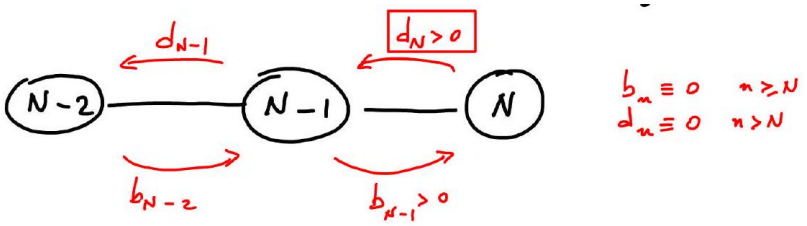
This is called the master equation of the birth-death process or generation-recombination process.

A few observations:

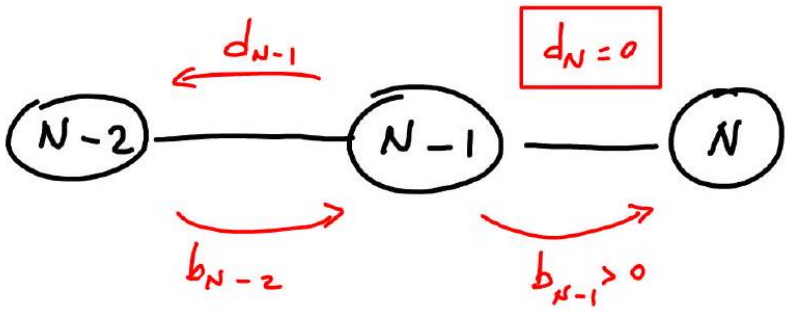
1. The M.E. is a gain-loss equation for the probabilities p_n;
2. We have to equip eq. (1) with initial conditions. If We start with $P_{n,n_0}(t_0) = \delta_{n,n_0}$, then the M.E. is the equation of the propagator of the Markov process, that is

$$P_n(t) \equiv P(n, t \mid n_0 t_0) \tag{0.177}$$

   So one can show (exercise) that $p_n(t)$ satisfies the Chapman-Kolmogorov eq. in its differential form. More follows on this.
3. We can introduce boundary conditions as well. For instance, if N is a reflecting boundary,



then $b_n \equiv 0 \forall n \geqslant N, d_n \equiv 0 \forall n > N$ (for $n < N, b_n$ and d_n are $\geqslant 0$) therefore if the state N is reached, it can be left from one side only. N is a reflecting state.
If N is an absorbing boundary,



here $d_N = 0$ which is important, because when the state N is reached, it can no longer be left. We say that N is an absorbing state.

Warning:

Because of the b.c. We have to be careful with eq. (1) as it holds only when the boundary states are not hit, otherwise it must be changed.

4. Notice that eq. (1) is linear and deterministic; indeed we can define a matrix $\mathbb{W}$ whose entries are

$$\mathbb{W}_{mm'} = d_{m'}\delta_{m,m'-1} + b_{m'}\delta_{m,m'+1} - (d_m + b_m)\,\delta_{m,n'} \quad (0.178)$$

So, if we introduce the vector notation $[\vec{p}(t)]_n \equiv p_n(t)$ we can write eq. (1) as

$$\begin{cases} \dot{\vec{P}}(t) = \mathbb{W}\vec{P} \\ \vec{P}(0) = \vec{P}_0 \end{cases} \quad (0.179)$$

and formally the solution reads $\vec{P}(t) = e^{\mathbb{W}t}\vec{P}_0$. The master equation defined in eq. (4b) holds in general for a continuous time, discrete Markov process as long as $\mathbb{W}$ satisfies the following properties:

a) $W_{nn'} \geqslant 0$ for $n \neq n'$
b) $\sum_m \mathbb{W}_{mn'} = 0$ for each n' (no abs. bound.)

The equations for the mean and the variance

From eq. (1) one can simply derive the eqs. for the time evolution of the mean and the variance. We first multiply eq. (1) by n and sum over n:

$\langle n \rangle \equiv \sum_{-\infty}^{+\infty} n p_n(t)$

$$\begin{aligned}\frac{d}{dt}\langle n \rangle &= \sum_{-\infty}^{+\infty} \left(n b_{n-1} p_{n-1} - n b_n p_n + n d_{n+1} p_{n+1} - n d_n p_n \right) \\ &= \sum_n \left[(n+1) b_n p_n - n b_n p_n + (n-1) d_n p_n - n d_n p_n \right] \\ &= \sum_n \left(b_n - d_n \right) p_n \end{aligned} \tag{0.180}$$

$$\frac{d}{dt}\langle n \rangle = \langle b_n \rangle - \langle d_n \rangle \qquad \begin{matrix} \langle b_n \rangle \equiv \sum_n b_n p_n \\ \langle d_n \rangle \equiv \sum_n d_n p_n \end{matrix} \tag{0.181}$$

with some initial conditions. Notice that this equation has to be equipped with different equations if there is an absorbing or reflecting b.c. Can you find them?

For the evolution of the variance we have to derive an equation for the second moment $\langle n^2 \rangle$. We first multiply eq. (1) by n^2 and then sum over n:

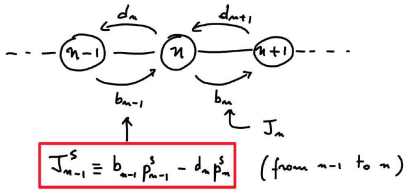
$$\begin{aligned}\frac{d}{dt}\langle n^2 \rangle &= \sum_{-\infty}^{+\infty} n^2 \left(b_{n-1} p_{n-1} + \cdots \right) = \\ &= \sum_n \left((n+1)^2 - n^2 \right) b_n p_n + \sum_n \left[(n-1)^2 - n^2 \right] d_n p_n \\ &= \sum_n (2n+1) b_n p_n + \sum_n (-2n+1) d_n p_n \\ &= 2 \sum_n n \left(b_n - d_n \right) p_n + \sum_n \left(b_n + d_n \right) p_n \end{aligned} \tag{0.182}$$

Thus

$$\frac{d}{dt}\langle n^2 \rangle = 2 \langle n \left(b_n - d_n \right) \rangle + \langle b_n + d_n \rangle \tag{0.183}$$

The equilibrium distribution

For birth and death process it is possible to calculate the equilibrium distribution of eq. (1) in general. This is not possible for more complicated discrete Markov processes. We will calculate the distribution for a b/d process defined between 0 (ref. b.c.) and ∞. We can define a stationary flux from $n-1$ to n:



From eq. (1) we get then

$$0 = \underbrace{b_{n-1} p^s_{n-1} - d_n p^s_n}_{J_{n-1}} + \underbrace{d_{n+1} p^s_{n+1} - b_n p^s_n}_{-J_n} \tag{0.184}$$

hence $J_n = J_{n-1} = \ldots = J_0 = b_{-1}p^s_{-1} - d_0 p^s_0 = 0$ (ref. b.c. at $n = 0$) then

$$J_n = b_{n-1}p^s_{n-1} - d_n p^s_n = 0 \Rightarrow b_{n-1}p^s_{n-1} = d_n p^s_n \quad \text{DETAILED BALANCE}$$
$$p^s_n = \frac{b_{n-1}}{d_n}p^s_{n-1} = \frac{b_{n-1}}{d_n}\frac{b_{n-2}}{d_{n-1}}p^s_{n-2} = \ldots \tag{0.185}$$

$$p^s_n = \prod_{i=1}^{n}\frac{b_{i-1}}{d_i}p^s_0 \quad \text{for } n = 1, 2, \ldots \tag{0.186}$$

because of normalization, $\left(p^s_0\right)^{-1} = 1 + \sum_{n=1}^{\infty}\prod_{i=1}^{n}\frac{b_{i-1}}{d_i}$; p^s_n exists if $p^s_0 < \infty$. The same approach can be used for a finite number of states $n = 1, \ldots, N$.

Simple yet important birth and death processes

Poisson process

This process is defined by the rates $b_n = \lambda, d_n = 0$, where $n = 0, 1, \ldots$ So the M.E. is

$$\begin{cases} \dot{p}_n = \lambda\left(p_{n-1} - p_n\right) \\ p_n(0) = \delta_{n,0} \end{cases} \tag{0.187}$$

Ex: show that the mean satisfies the eq. $\frac{d}{dt}\langle n\rangle = \lambda$ and so $\langle n(t)\rangle = n_0 + \lambda t$ if $p_n(0) = \delta_{n,n_0}$.

We solve eq. (8) with the method of the generating function:

$$g(z,t) \equiv \sum_{n=0}^{\infty} z^n p_n(t) \tag{0.188}$$

So from eq. (8) we get an eq. for g:

$$\begin{cases} \frac{\partial}{\partial t}g(z,t) = \lambda(z-1)g(z,t) \quad \left(g(1,t) = \sum_n p_n(t) = 1\right) \\ g(z,0) = \sum_n z^n \delta_{n,0} = 1 \end{cases} \tag{0.189}$$

The solution of (9) is then

$$g(z,t) = e^{\lambda(z-1)t} = e^{-\lambda t}\sum_{n=0}^{\infty}\frac{(\lambda t)^n}{n!}z^n \tag{0.190}$$

hence

$$p_n(t) = e^{-\lambda t}\frac{(\lambda t)^n}{n!} \tag{0.191}$$

Show that $\mathrm{var}(n(t)) = \lambda t$.

Radioactive decay

Initially the system consists of N_0 radioactive particles which decay at rate γ. Therefore, if at time t there are n surviving particles, then in the following Δt time the probability of one decay is $\gamma n \Delta t$ and more than

one decay is $o(\Delta t)$. Thus $d_n = \gamma n$ and $b_n = 0$ and the M.E. is

$$\begin{cases} \dot{p}_n = \gamma(n+1)p_{n+1}(t) - \gamma n p_n(t) \quad n = 0, 1 \dots N_0 - 1 \quad \text{a.b.c. at } n = 0. \\ \dot{p}_{N_0} = -\gamma N_0 p_{N_0}(t) \\ p_n(0) = \delta_{n,N_0} \end{cases} \tag{0.192}$$

Ex: show that $\frac{d}{dt}\langle n \rangle = -\gamma \langle n \rangle$, so $\langle n(t) \rangle = N_0 e^{-\gamma t}$. With the generating function $g(z,t) = \sum_{n=0}^{N_0} z^n p_n(t)$ we get

$$\frac{\partial g(z,t)}{\partial t} = \gamma(1-z)\frac{\partial}{\partial z} g(z,t) \quad \begin{matrix} g(1,t) = 1 \\ g(z,0) = z^{N_0} \end{matrix} \tag{0.193}$$

Notice that $h(z,t) = \varepsilon(t)(1-z)+1$ leads to $\dot{\varepsilon} = -\gamma\varepsilon$, namely $\varepsilon(t) = \varepsilon_0 e^{-\gamma t}$, so $h(1,t) = 1$, but $h(z,0) = \varepsilon_0(1-z) + 1 \neq z^{N_0}$. However, take g as a function of h, i.e. $g(z,t) = f(h(z,t))$, we get from (11)

$$\frac{\partial g}{\partial t} = \frac{df}{dh}\frac{\partial h}{\partial t} \quad , \quad \frac{\partial g}{\partial z} = \frac{df}{dh}\frac{\partial h}{\partial z} \tag{0.194}$$

and $\frac{df}{dh}$ simplifies, because it occurs on both sides of eq. (11). We can then use f to satisfy the i.c.: $f(a) = a^{N_0}$ does the job. We take $g = \left(\varepsilon_0 e^{-\gamma t}(1-z) + 1\right)^{N_0}$ where $\varepsilon_0 = -1$. Eventually, the sol, is

$$g(z,t) = \left(e^{-\gamma t}(z-1) + 1\right)^{N_0} \tag{0.195}$$

We have now to invert this relation to get $p_n(t)$

$$g(z,t) = \left(e^{-\gamma t} z + \left(1 - e^{-\gamma t}\right)\right)^{N_0} = \sum_{n=0}^{N_0} \binom{N_0}{n} \left(1 - e^{-\gamma t}\right)^{N_0 - n} e^{-n\gamma t} z^n \tag{0.196}$$

which gives

$$p_n(t) = \binom{N_0}{n} e^{-n\gamma t} \left(1 - e^{-\gamma t}\right)^{N_0 - n} \tag{0.197}$$

We can interpret this eq. in this way: $e^{-n\gamma t}$ is the prob. that n particles have survived (i.e., not decayed yet) by time t, $\left(1 - e^{-\gamma t}\right)^{N_0 - n}$ is the prob. that $N_0 - n$ particles have decayed by time t. We also need the factor $\binom{N_0}{n}$ because the specific identity of the particles is not important, then there are $\binom{N_0}{n}$ ways to select n surviving particles out of N_0.

Furry process

A cosmic electron enters an absorbing material (like lead...) and branches into multiple particles (an electron may emit a photon which may then produce an $e^+ - e^-$ pair). So a cascade of secondary particles is produced which generates a shower of final particles. This process can be described by a birth and death process where $b_n = \gamma n$ and $d_n = 0, n = 1, 2, \dots$ The M.E. is then

$$\begin{cases} \dot{p}_n = \gamma(n-1)p_{n-1} - \gamma n p_n \\ p_n(0) = \delta_{n,1} \end{cases} \tag{0.198}$$

Show as before that

$$\begin{aligned} \langle n(t) \rangle &= e^{\gamma t} \\ \mathrm{Var}(n(t)) &= e^{\gamma t} \left(e^{\gamma t} - 1 \right) \end{aligned} \tag{0.199}$$

Finally:

$$p_n(t) = e^{-\gamma t} \left(1 - e^{-\gamma t} \right)^{n-1} \tag{0.200}$$

try to interpret the result.

The contact process

Let us assume that a population of N individuals can be divided into two categories according to whether they are infected or not (but are susceptible any way). If an indiv. has not yet caught the infection, may catch it from any of of the n infected ones (uniformly at random). We can write down the transition rate from n to $n+1$ infected individuals; if the number of infected ind. increases by one, then one healthy ind. must get in contact with an infected one:

1. first, we have to pick one healthy indiv.

$$b_n = \tilde{\beta} \tfrac{N-n}{N} \tfrac{n}{N-1} = \tfrac{\beta}{N} n(N-n) \tag{0.201}$$

2. second, the healthy ind. have to encounter an infected one.

We then assume that an infected individual recovers at rate γ. then the transition rate from state n to $n-1$ is $d_n = \gamma n$. Notice that $b_0 = 0 = d_0$ ($n = 0$ is an absorbing state) and $b_N = 0, d_N \neq 0$ ($n = N$ is a reflecting state) and we have to set $d_{N+1} = 0$. Notice that the rates b_n and d_n can be written as a function of $x = \frac{n}{N} : b_x = N\beta x(1-x), d_x = N\gamma x$. As N becomes large, the variations in n become small and so one hopes to describe x as a continuous variable. Making this limit rigorous is tricky (Kurtz's theorem), but one can anyway guess the limiting equation. the important assumption is the existence of a typical scale of the system (in this case N) and that the parameters (here β and γ) scale appropriately with N.

The master equation has a form

$$\dot{q}_n(t) = b_{\frac{n-1}{N}} q_{n-1} + d_{\frac{n+1}{N}} q_{n+1} - \left(b_{\frac{n}{N}} + d_{\frac{n}{N}} \right) q_n \tag{0.202}$$

In the continuous limit $q_n(t)$ becomes a PDF of x, so we write

$$q_n(t) = \frac{1}{N} p(x,t) \quad \text{for large } N \tag{0.203}$$

So eq. (15) becomes

$$\dot{p}(x,t) = b_{x-\frac{1}{N}} p\left(x - \frac{1}{N}, t \right) + d_{x+\frac{1}{N}} p\left(x + \frac{1}{N}, t \right) - (b_x + d_x) p(x,t) \tag{0.204}$$

As $\frac{1}{N}$ is small, we can Taylor expand eq. (16):

$$\begin{aligned} b_{x-\frac{1}{N}}\, p\left(x-\frac{1}{N}\right) - b_x p(x) &= -\frac{1}{N}\frac{d}{dx}\left(b_x p_x\right) + \frac{1}{2}\frac{1}{N^2}\frac{d^2}{dx^2}\left(b_x p_x\right) + \text{ h.o.t.} \\ d_{x+\frac{1}{N}}\, p\left(x+\frac{1}{N}\right) - d_x p(x) &= \frac{1}{N}\frac{d}{dx}\left(d_x p_x\right) + \frac{1}{2}\frac{1}{N^2}\frac{d^2}{dx^2}\left(d_x p_x\right) + \text{ h.o.t.} \end{aligned} \tag{0.205}$$

Therefore

$$\dot{p}(x,t) = -\frac{1}{N}\frac{\partial}{\partial x}\left[\left(b_x - d_x\right)p_x\right] + \frac{1}{2N^2}\frac{\partial^2}{\partial x^2}\left[\left(b_x + d_x\right)p_x\right] + \text{ h.o.t.} \tag{0.206}$$

as $b_x = N\beta x(1-x)$ and $d_x = N\gamma x$ we get the F.P. equation

$$\dot{p}(x,t) = -\frac{\partial}{\partial x}[(\beta x(1-x) - \gamma x)p] + \frac{1}{2N}\frac{\partial^2}{\partial x^2}[(\beta x(1-x) + \gamma x)p] \tag{0.207}$$

which corresponds to an Itô SDE: $(0 < x < 1)$

$$dx = (\beta x(1-x) - \gamma x)dt + \sqrt{\frac{\beta x(1-x) + \gamma x}{N}}dB(t) \tag{0.208}$$

Fluctuations are of order $N^{-1/2}$.

In general, although the equation and its derivation are not rigorous, a birth and death process may be well approximated by the F.P. equation

$$\dot{p}(x,t) = -\frac{\partial}{\partial x}\left[\left(b_x - d_x\right)p_x\right] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[\left(b_x + d_x\right)p_x\right] \tag{0.209}$$

at least in some region of the parameter space. It is anyway expected that eq. (19) is very inaccurate close to (possible) boundaries or when N (or other typical param.) is small. This approx is called Kramers-Moyal expansion and has several generalizations. Other more rigorous approximations exist (like the van Kampen approximation (see p. 244, van Kampen) or the WKB expansion... which are more accurate but more difficult as well.

Back to the contact process. The mean of the infected individuals, $\rho(t) \equiv \mathbb{E}(x(t))$, satisfies (see eq. (18b))

$$\dot{\rho} = (\beta - \gamma)\rho - \beta\mathbb{E}\left(x(t)^2\right) \tag{0.210}$$

This equation is not closed and cannot be solved, unless we know the behavior of $\mathbb{E}\left(x^2\right)$. The mean depends on the fluctuations. However, the eq. for $\mathbb{E}\left(x^2\right)$ depends on $\mathbb{E}\left(x^3\right)$, so we obtain an infinite chain of equations which cannot be solved unless we solve the full F.P. equation. One way to obtain some information is to resort to the moment closure: if fluctuations are small, then

$$\mathbb{E}\left(x^2(t)\right) \simeq \mathbb{E}(x(t))^2 = \rho(t)^2 \tag{0.211}$$

Under this approximation

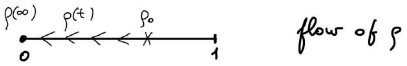
$$\dot{\rho} = (\beta - \gamma)\rho - \beta\rho^2 \tag{0.212}$$

which is a logistic equation that can be solved as we have seen at the beginning of the course. There are two steady states ($\dot{\rho} = 0$): $\rho^* = 0$ and

$\bar{\rho} = \frac{\beta-\gamma}{\beta}$. What is their meaning? Let's look at their stability:

$$\frac{d\dot{\rho}}{d\rho} = \beta - \gamma - 2\beta\rho\Big|_{\rho=\rho^{st}} = \begin{cases} \beta-\gamma & \rho = \rho^* = 0 \\ \gamma-\beta & \rho = \bar{\rho} = \frac{\beta-\gamma}{\beta} \end{cases} \tag{0.213}$$

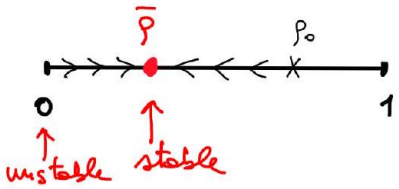
- Therefore $\rho = 0$ is stable as $\beta < \gamma$ (and $\bar{\rho}$ is unstable)



after some time, the eq. is well approximated by

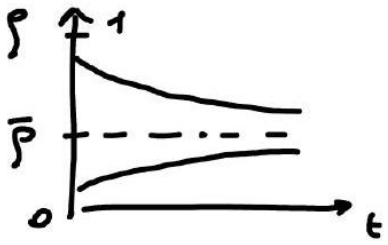
$$\dot{\rho} = (\beta-\gamma)\rho \quad \to \rho(t) = \tilde{\rho}e^{-|\beta-\gamma|t}\rho \to_t \tag{0.214}$$

- Viceversa, $\bar{\rho} = \frac{\beta-\gamma}{\beta} (> 0)$ is stable as $\beta > \gamma$ (and $\rho = 0$ is unstable)



after some time, the eq. is well approximated by $\rho(t) = \bar{\rho} + y(t)$ $(y \ll \bar{\rho})$

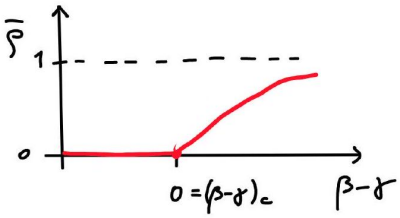
$$\dot{\rho} = -(\beta-\gamma)(\bar{\rho}-\rho) \quad \to \quad \rho(t) = \bar{\rho} + \tilde{\rho}e^{-|\beta-\gamma|t} \tag{0.215}$$



So the characteristic time scale is $|\beta-\gamma|^{-1}$ in both cases. Of course this is summarized by the full solution:

$$\rho(t) = \frac{\bar{\rho}}{1 + \left(\frac{\bar{\rho}}{\rho_0} - 1\right) e^{(\gamma-\beta)t}} = \frac{(\beta-\gamma)\rho_0}{\beta\rho_0 + \left(\beta - \gamma - \beta\rho_0\right) e^{(\gamma-\beta)t}} \tag{0.216}$$

where ρ_0 is the initial condition for the density $(0 < \rho_0 < 1)$ of infected individuals. The phase diagram of this process reads:



$$\begin{gathered}\bar{\rho} \sim (\beta - \gamma)^1 \\ \beta > \gamma\end{gathered} \tag{0.217}$$

At the critical point $\beta = \gamma$:

$$\dot{\rho} = -\beta\rho^2 \quad \rightarrow \quad \rho(t) = \frac{\rho_0}{1+\beta t} \sim \frac{1}{t} \quad t \gg \beta^{-1} \tag{0.218}$$

the decay is no longer exponential but power law: critical slowing down.

Exercise: the discrete random walk in continuous time is governed by the master equation (symmetric R.W.)

$$\dot{p}_n = p_{n+1} + p_{n-1} - 2p_n \quad p_n(0) = \delta_{n,0} \tag{0.219}$$

Show that the generating function $F(z,t) = \sum_{-\infty}^{+\infty} z^n p_n(t)$ satisfies

$$\dot{F} = \left(z + \frac{1}{z} - 2\right) F \tag{0.220}$$

so the solution is $F(z,t) = \exp\left[t\left(z + z^{-1} - 2\right)\right]$. From this find

$$p_n(t) = e^{-t} \sum_{\substack{l \geqslant 0 \\ l+m \geqslant 0}} \frac{t^{2l+m}}{(l+m)!l!} \tag{0.221}$$

Find the K.M. expansion of the M.E. and find its solution.

A simple chemical reaction

Consider the reaction

$$X \underset{k_2}{\overset{k_1}{\rightleftarrows}} A \tag{0.222}$$

where the product A is not affected by x and it does not decrease its quantity even though it produces particles at rate k_2. We are interested into the stochastic evolution of X: the r.v. n. From a simple application of the mass action law we get the evolution of the deterministic value $\rho(t) = \mathbb{E}(n(t))$:

$$\dot{\rho} = -k_1\rho + k_2 a \tag{0.223}$$

where a is a constant.

We want now to get information about the fluctuations: If at time t there are n particles of type x, then the prob. that at time $t + \Delta t$ there is one more is given by $k_2 a \Delta t$, and one less is $k_1 n \Delta t$. So we get a birth and death process with rates

$$\begin{aligned} b_n &= k_2 a \equiv b \quad (\text{ a constant }) \\ d_n &= k_1 n \end{aligned} \tag{0.224}$$

where $n = 0, 1, \ldots$ It is not difficult to find that the equilibrium distribution

of n (from eq. (7))

$$p_n^{st} = \frac{\lambda^n}{n!} e^{-\lambda} \quad \lambda = \frac{k_2 a}{k_1} \tag{0.225}$$

what is the difference between this solution and eq. (10)? The average is also (from eq. (5))

$$\frac{d}{dt}\langle n \rangle = b - k_1 \langle n \rangle \tag{0.226}$$

which is like eq. 23. Ex: find the M.E. for the chemical reaction $A + x \xrightarrow{k_1} 2x, x \underset{k_3}{\overset{k_2}{\rightleftarrows}} B$. and compare the results with those from the law of mass action.

Exact simulation of a birth and death process: the Gillespie's algorithm

The M.E. in eq. (1) governs a b/d process whose trajectories can be generated exactly (up to machine numerical errors). The M.E. includes all the info we need as it defines the process itself. We know that it is a Markov process therefore the information that we possess at time t is enough to define what happens in the future. We need two pieces of info to generate a path:

1. What is the time of the next event (either birth or death)?
2. What is the nature of the event, given that it occurs? namely, what is the probability that it is a birth/death?

If we can answer these two questions then we know when and how the path changes. Let's define $q_0(\tau \mid n)$ as the probability that no events will occur within the interval $[0, \tau)$, given that the system was in the state n at time $t = 0$ (as the process is homogeneous, $t = 0$ is not a restrictive assumption). Notice that if T is the (random) time when the next event (birth or death) will occur, then $q_0(\tau \mid n) = P(T > \tau \mid n)$. We build up an equation for $q_0(\tau \mid n)$ by using the Markov assumption and that the process is a b/d process: The prob. that there are no events in the interval $[0, \tau + \Delta\tau)$ is given by the prob. that no events occur within $[0, \tau)$ and neither occur in $[\tau, \tau + \Delta\tau)$:

$$q_0(\tau + \Delta\tau \mid n) = q_0(\tau \mid n)\,(1 - b_n \Delta\tau - d_n \Delta\tau) \tag{0.227}$$

Therefore as $\Delta\tau \to 0$

$$\begin{cases} \dfrac{dq_0(\tau \mid n)}{d\tau} = -\,(b_n + d_n)\, q_0(\tau \mid n) \\ q_0(0 \mid n) = 1 \end{cases} \tag{0.228}$$

hence

$$q_0(\tau \mid n) = e^{-(b_n + d_n)\tau} \tag{0.229}$$

Now we can calculate $q_+(\tau \mid n)\Delta\tau$, namely, the probability that a birth occurs between τ and $\tau + \Delta\tau$ if the system was in state n. This is simply

$$q_+(\tau \mid n)\Delta\tau = e^{-(b_n+d_n)\tau} b_n \Delta\tau \tag{0.230}$$

prob. of no events up to time τ prob. of 1 birth event between τ and $\tau + \Delta\tau$

Therefore the PDF is

$$q_+(\tau \mid n) = b_n e^{-(b_n+d_n)\tau} \tag{0.231}$$

and for a death event

$$q_-(\tau \mid n) = d_n e^{-(b_n+d_n)\tau} \tag{0.232}$$

and the PDF of any event (either birth or death) is therefore

$$q_1(\tau \mid n) = (b_n + d_n)\, e^{-(b_n+d_n)\tau} \tag{0.233}$$

This means that the PDF of an event is exponentially distributed with mean time $\langle \tau(n) \rangle = (b_n + d_n)^{-1}$ (show this). Of course, we assume that the state n is not absorbing, i.e. $b_n + d_n > 0$.

Now $q_+(\tau \mid n)\Delta\tau = \left(\begin{array}{c} \text{prob. of a birth event,} \\ \text{given that an event occurs} \\ \text{between } \tau \text{ and } \tau + \Delta\tau \end{array} \right) \left(\begin{array}{c} \text{prob. that an event occurs} \\ \text{between } \tau \text{ and } \tau + \Delta\tau \end{array} \right)$

From eqs. (27) we get

$$q_+(\tau \mid n)\Delta\tau = \frac{b_n}{b_n + d_n} (b_n + d_n)\, e^{-(b_n+d_n)\tau} \Delta\tau \tag{0.234}$$

prob. of a birth event, given that an event occurs between τ and $\tau + \Delta\tau$ when the state is n prob. that an event occurs (birth or death) between τ and $\tau + \Delta\tau$ when the state is n

Eq. (30) suggests an algorithm for simulating a path from the master equation (1):

Gillespie's algorithm

(1) Initialize the system at time $t = 0$, starting at state n_0: (2) If $b_n + d_n > 0$, generate the time τ when the next event will occur. So you have to draw a random number from the exponential distribution (29), or equivalently (show this)

$$\tau = \frac{1}{b_n + d_n} \ln\left(\frac{1}{r}\right) \tag{0.235}$$

Where r is a random number uniformly distributed in $(0, 1)$. Update the time

$$t_{\text{new}} = t_{\text{old}} + \tau \tag{0.236}$$

t_{old} is the time when the state was n;

If $b_n + d_n = 0$, stop the program as t_{old} is the extinction time and n is an absorbing state. (3) Compute whether the next event will be a birth or a death.

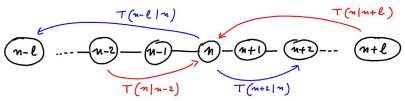
As before, let n be the state at time t_{old} . If $b_n + d_n > 0$, generate a random number u uniformly distributed in $(0, 1)$.

- According to eq. (30), if $u < \frac{b_n}{b_n + d_n}$, then the next event will be a birth. Update the state $n_{\text{new}} = n + 1$
- Otherwise, the next event will be a death so the update is $n_{\text{new}} = n - 1$. Of course, if $b_n + d_n = 0$ there cannot be any further update and n is the final absorbing state.

(4) Repeat the steps (2) and (3) as needed.

More general discrete Markov processes

It is not difficult to generalize the considerations that we used for the birth and death processes to continuous time Markov processes where multiple jumps are allowed. Calculation are more difficult but the conceptual framework is similar. The M.E. can be deduced from the Chapman-Kolmogorov equation, but it can also be guessed as we did. Take $n \in E \subseteq \mathbb{Z}$. Let $T(n' \mid n)\,\Delta t$ be the probability to jump to state $n'(\neq n)$ at time $t + \Delta t$, given that the system was in state n at time t. So $T(n' \mid n) \geqslant 0$ is the corresponding jumping rate. T could depend on time t, but we consider the simpler case in which it does not. We can visualize this as follows



The M.E. for the propagator $p(n, t \mid n_0, t_0)$ is then

$$P(n, t + \Delta t) = \underbrace{\sum_{m \neq n} T(n \mid m)\Delta t}_{\substack{\text{probability to} \\ \text{jump from any state } m \neq n \\ \text{into the state } n}} P(m, t) + \underbrace{\left(1 - \sum_{m \neq n} T(m \mid n)\Delta t\right)}_{\substack{\text{probability to} \\ \text{remain in the state } n}} P(n, t) \tag{0.237}$$

Therefore as $\Delta t \longrightarrow 0$ the Master Equation becomes

$$\frac{\partial}{\partial t} p(n, t) = \sum_m [T(n \mid m)p(m, t) - T(m \mid n)p(n, t)] \tag{0.238}$$

notice that we have included the state n in the sum (why?).

As usual eq. (31) must be equipped with initial conditions $P(n, t_0 \mid n_0, t_0) = \delta_{n,n_0}$ and, possibly, some boundary conditions.

Exercise: - Show that $\sum_n p(n, t) = 1$.

- Define the l-th jump moment as

$$\mu_l(n) = \sum_m (m - n)^l T(m \mid n) \quad l \geqslant 0 \tag{0.239}$$

Show then that

$$\frac{d}{dt}\langle n\rangle = \left\langle \mu_1(n)\right\rangle \rightarrow \text{ is this a closed eq. for } \langle n\rangle \text{ ?} \quad (0.240)$$

$$\frac{d}{dt}\left\langle n^2\right\rangle = \left\langle \mu_2(n)\right\rangle + 2\left\langle n\mu_1(n)\right\rangle \quad (0.241)$$

where $\langle f(n)\rangle \equiv \sum_n f(n)p(n,t)$

As we have seen in eq. (4a) and (4b), we can define a matrix $\mathbb{W}$ whose entries are ($T(n \mid n) = 0$)

$$W_{nm} = T(n \mid m) - \sum_l T(l \mid n)\delta_{n,m} \quad (0.242)$$

which shows that $\mathbb{W}_{nm} \geq 0$ for $n \neq m$ and $\sum_n \mathbb{W}_{nm} = 0$. The M.E. eq. (31) then reads

$$\dot{\vec{p}} = W\vec{p} \quad \text{or} \quad \dot{p}_n = \sum_m \mathbb{W}_{nm}p_m$$

$$\mathbb{W} = \begin{pmatrix} w_{11} & T(1\mid 2) & T(1\mid 3) & \dots \\ T(2\mid 1) & w_{22} & T(2\mid 3) & \dots \\ T(3\mid 1) & T(3\mid 2) & w_{33} & \\ \vdots & \vdots & & \ddots \end{pmatrix} \leftarrow \text{ jumps from } m = 2, 3\dots \text{ to } 1 \quad (0.243)$$

$$w_{ii} \equiv -\sum_{\substack{m \\ \text{jumps from} \\ 1 \text{ to } m=2,3,\dots}} T(m \mid i)$$

We can find the stationary state by setting $\dot{P}_n = 0$ From eq. (31):

$$\sum_m \left[T(n \mid m)p_{st}(m) - T(m \mid n)p_{st}(n)\right] = 0 \quad (0.244)$$

This eq. is difficult to solve in general. However we can find the equilibrium solution if each and every term in the sum is zero (much stronger assumption). In this latter case we get

$$T(n \mid m)P_{eq}(m) = T(m \mid n)P_{eq}(n) \quad \text{DETAILED BALANCE} \quad (0.245)$$

This assumption means that every state m is balanced only by the state n, like in the birth and death case, which in general is not true. All states are balanced in pairs. Of course, the detailed balance condition satisfies eq. (32), but eq. (32) does not imply eq. (33). In general one cannot impose eq. (33).

We again can connect this to stat. Mech. If

$$P_{\text{eq.}}(n) = \frac{1}{z}e^{-\beta E(n)} \quad (0.246)$$

Where $E(n)$ is the energy of state n, then eq. (32) is satisfied if we choose $T(n \mid m)$ and $T(m \mid n)$ such that

$$\frac{T(n \mid m)}{T(m \mid n)} = e^{-\beta(E(n)-E(m))} \quad (0.247)$$

Even though other choices are possible to satisfy detailed balance, eq. (33) allows us to describe a physical system at equilibrium with a heat

bath at temperature β^{-1}.

Gaussian Integrals **First Semester**

Lecture 6

Date: 2025-10-01 Profesor: Azaele Sandro

0.6 Gaussian Integrals

Let's consider the Gaussian distribution (PDF):

$$p(x) = ce^{-\frac{ax^2}{2}} \quad a > 0 \tag{0.248}$$

$p(x)$ must be normalized in $(-\infty, +\infty)$, so

$$\int_{-\infty}^{+\infty} p(x)dx = 1 \quad \Rightarrow \quad c\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}}dx = 1 \tag{0.249}$$

This gives the simplest form of Gaussian integral:

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}}dx = \sqrt{\frac{2\pi}{a}} \quad a > 0 \tag{0.250}$$

A more general Gaussian integral:

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}+bx}dx = ? \tag{0.251}$$

To solve it we use a change of vars. Notice that the min. of the exponent has changed.

$$\frac{d}{dx}\left(-\frac{ax^2}{2} + bx\right) = -ax + b = 0 \quad \Rightarrow \quad x = \frac{b}{a} \quad b \in \mathbb{R} \tag{0.252}$$

We introduce the new var. $y = x - \frac{b}{a}$. We sub this into the exponent:

$$-\frac{ax^2}{2} + bx = -\frac{a}{2}\left(y + \frac{b}{a}\right)^2 + b\left(y + \frac{b}{a}\right) = -\frac{a}{2}\left(y^2 + \frac{2by}{a} + \left(\frac{b}{a}\right)^2\right) + by + \frac{b^2}{a} = \tag{0.253}$$
$$= -\frac{a}{2}y^2 + \frac{b^2}{2a}$$

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}+bx}dx = \int_{-\infty}^{+\infty} e^{-\frac{ay^2}{2}+\frac{b^2}{2a}}dy = e^{\frac{b^2}{2a}}\int_{-\infty}^{+\infty} e^{-\frac{ay^2}{2}}dy \Rightarrow$$

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}+bx}dx = \sqrt{\frac{2\pi}{a}}e^{\frac{b^2}{2a}} \quad a > 0 \tag{0.254}$$

Let's calculate the integral in eq. (3) when $b = it, t \in \mathbb{R}$.

$$\varphi(t) = \int_{-\infty}^{+\infty} dx e^{ixt}\sqrt{\frac{a}{2\pi}e^{-\frac{ax^2}{2}}} \tag{0.255}$$

This is the Fourier transform of the Gaussian PDF, which is also the characteristic function of the Gaussian PDF.

We take the time derivative of φ:

$$\varphi'(t) = \sqrt{\frac{a}{2\pi}}i\int dx \times e^{ixt}e^{-\frac{a}{2}x^2} \tag{0.256}$$

Why can we do this? In general, $\frac{d}{dt}\int f(x,t)dx = \int \frac{\partial}{\partial t}f(x,t)dx$ if $f, \partial_t f$ are continuous and uniformly bounded, which means $|f(x,t)| <$

$A(x), \left|\partial_t f(x,t)\right| < B(x)$ where $\int A(x)dx < \infty \int B(x)dx < \infty$.

$$\begin{aligned}
\varphi'(t) &= \sqrt{\frac{a}{2\pi}} i \int dx \times e^{ixt} e^{-\frac{a}{2}x^2} \\
&= -\frac{i}{\sqrt{2\pi a}} \int dx e^{ixt} \frac{d}{dx} e^{-\frac{ax^2}{2}} \quad \frac{d}{dx} e^{-\frac{ax^2}{2}} = -axe^{-ax^2/2} \\
&= -\frac{t}{\sqrt{2\pi a}} \int_{-\infty}^{+\infty} dx e^{ixt} e^{-\frac{ax^2}{2}} \\
&= -\frac{t}{a}\varphi(t)
\end{aligned} \tag{0.257}$$

So $\varphi' = -\frac{t}{a}\varphi(t)$ and the solution is $\varphi(t) = ce^{-\frac{t^2}{2a}}$ (check this out!). However as $\varphi(0) = 1 \Rightarrow c = 1$,

$$\varphi(t) = e^{-\frac{t^2}{2a}} \tag{0.258}$$

If we set $b = it$, we get $e^{\frac{b^2}{2a}} = e^{-\frac{t^2}{2a}}$, which is consistent.

Wiener path integral **First Semester**

Lecture 7

Date: 2025-10-17 Profesor: Azaele Sandro

0.7 Wiener path integral

The Wiener measure and the Wiener path integral (Techniques and Applications of Path Integration by L.S. Schulman) We have seen that the propagator of the Brownian motion satisfies the Chapman-Kolmogorov eq. because it is a Markov process. From eq. (13) and (11)

$$w(x_2,t_2 \mid x_0,t_0) = \int_{-\infty}^{+\infty} w(x_2,t_2 \mid x_1,t_1)\, w(x_1,t_1 \mid x_0,t_0)\, dx_1 \quad (0.259)$$

Notice the analogy with QM: $\langle x_2 t_2 \mid x_0 t_0\rangle = w(x_2 t_2 \mid x_0 t_0)$, we insert an identity $\int dx_1 \,|x_1,t_1\rangle\langle x_1,t_1| = 1$ and get $\langle x_2 t_2 \mid x_0 t_0\rangle = \int dx_1 \langle x_2 t_2 \mid x_1 t_1\rangle\langle x_1 t_1 \mid x_0 t_0\rangle$ We can also iterate eq. (14) n-times and get for $t_n > t_{n-1} > \ldots > t_1 > t_0$

$$w(x_n,t_n \mid x_0,t_0) = \int_{-\infty}^{+\infty} w(x_n,t_n \mid x_{n-1},t_{n-1}) \cdots w(x_1,t_1 \mid x_0,t_0)\, dx_{n-1} \ldots dx_1 \quad (0.260)$$

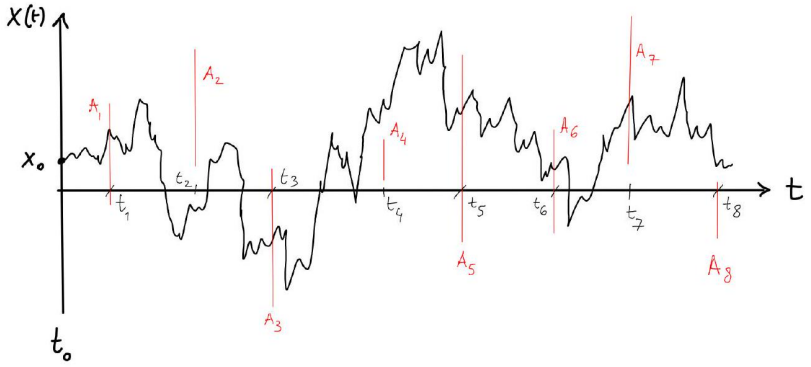
This is an important property of the propagator, because it allows us to understand what is the probability to find a Brownian particle in different regions at different times. Indeed, if we define the Wiener measure $t_n > t_{n-1} > \ldots > t_1 > t_0$

$$d\mathbb{P}_{t_1 \ldots t_n}(x_1 \ldots x_n \mid x_0,t_0) = \prod_{i=1}^{n} w(x_i,t_i \mid x_{i-1},t_{i-1})\, dx_i \quad (0.261)$$

then (interval $A_i \subseteq \mathbb{R}$)

$$\mathbb{P}(\{A\} \mid x_0,t_0) = \int_{A_n} \cdots \int_{A_1} w(x_n t_n \mid x_{n-1} t_{n-1}) \cdots w(x_1 t_1 \mid x_0 t_0)\, dx_{n-1} \ldots dx_1 \quad (0.262)$$

gives the joint probability to find a Brownian particle in the area A_1 at time t_1, within A_2 at time t_2 and within A_n at time t_n $(t_1 < t_2 \cdots < t_n)$, given that it started off at x_0 at time $t_0 < t_1$.



The explicit expression is $(\Delta t_i = t_i - t_{i-1} > 0)$

$$d\mathbb{P}_{t_1 \ldots t_n}(x_1 \ldots x_n \mid x_0,t_0) = e^{-\frac{1}{2D}\sum_{i=1}^{n} \frac{(x_i - x_{i-1})^2}{\Delta t_i}} \prod_{i=1}^{n} \frac{dx_i}{\sqrt{2\pi D \Delta t_i}} \quad (0.263)$$

This relation is valid for any $n \in \mathbb{N}$ and we can extend the result to any subset of the σ-algebra generated by the cylindrical sets of the form $A = \{x(t) : x(t_1) \in A_1, x(t_2) \in A_2 \ldots x(t_n) \in A_n\}$. When we take the

limit $n \to \infty$ we obtain the so called Wiener path integral. In this case

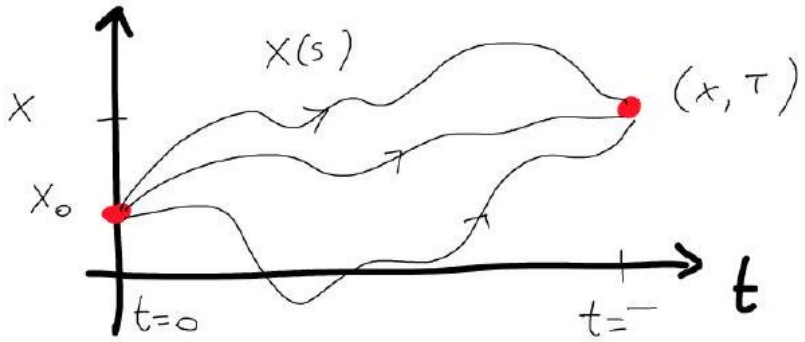
$$\sum_{i=1}^{n} \frac{(x_i - x_{i-1})^2}{\Delta t_i} = \sum_{i=1}^{n} \left(\frac{x_i - x_{i-1}}{\Delta t_i} \right)^2 \Delta t_i \xrightarrow[\substack{n\to\infty \\ \max(\Delta t_i)\to 0}]{\sum \Delta t_i = T} \int_0^T (\dot{x}(s))^2 ds \tag{0.264}$$

and eq. (16) gets the suggestive form

$$d\mathbb{P}_w \propto \prod_{\tau=0^+}^{T} dx(\tau) e^{-\frac{1}{2D}\int_0^T \dot{x}(s)^2 ds} \tag{0.265}$$

This formula is only formal as it does not exist (it is infinite!). However, it is very useful for calculating averages of functionals which are exponentials of quadratic expressions of the trajectory $x(s)$ or for approximations with the saddle point method. Another way to look at eq. (14b) is the following. We fix $x_n = x$, $t_n = T$ and x_0 at t_0. Then all the integrations $x_{n-1}, x_{n-2} \ldots, x_1$ at the corresponding ordered times $t_{n-1}, \ldots t_1$ show that in the limit $n \to \infty$ (with fixed $x, T; x_0, t_0$) the propagator of a Brownian particle $W(x, T \mid x_0, t_0)$ can be written as

$$w(x, T \mid x_0, t_0) = \int_{x(0)=x_0}^{x(T)=x} \mathcal{D}x(\tau) e^{-\frac{1}{2D}\int_0^T \dot{x}(s)^2 ds} = \int_{x(0)=x_0}^{x(T)=x} \mathcal{D}x(\tau) e^{-\frac{S[x(s)]}{D}} \tag{0.266}$$



the propagator W can be written as an integral over all trajectories between (t_0, x_0) and (T, x) of the Brownian particle.

Here $S[x(s)]$ is the action and $S = \int_0^T L[x] ds$, where L is the Lagrangian of the system. Here $L[x(s)] = \frac{1}{2D}\left(\frac{dx}{ds}\right)^2$ which can be interpreted as the kinetic energy of a free particle. Furthermore, notice that if we change variable $s = it/\hbar$ (as an analytic continuation), identify $D = \frac{\hbar^2}{m}$ and introduce the "imaginary" time $\tilde{t} = -i\hbar T$, then the propagator in (17b) becomes

$$W\left(x, \tilde{t} \mid x_0, 0\right) = \int_{x(0)=x_0}^{x(\tilde{t})=x} \mathcal{D}x\,(t')\, e^{\frac{i}{\hbar}\int_0^{\tilde{t}} \frac{1}{2}m\left(\frac{dx}{dt'}\right)^2 dt'} = \sqrt{\frac{m}{2\pi i\hbar\tilde{t}}}\, e^{\frac{im}{2\hbar\tilde{t}}(x-x_0)^2} \tag{0.267}$$

This is the propagator (or Green's function) of the Schrödinger eq:

$$i\hbar\frac{\partial\psi}{\partial t} = \hat{H}\psi \quad \text{where} \quad \hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} \tag{0.268}$$

we can write $W\left(x, \tilde{t} \mid x_0, 0\right) =$

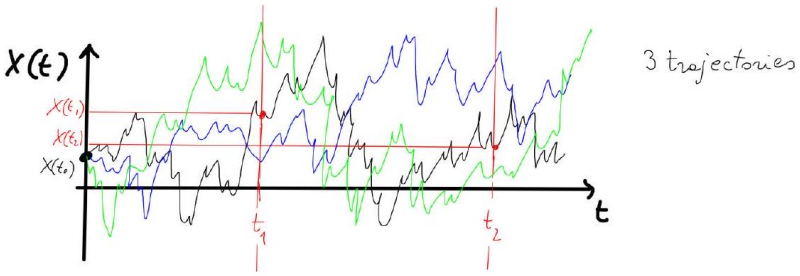
$langlex|e^{-\frac{i}{\hbar}\tilde{t}\hat{H}}|x_0\rangle$ and correspondingly we can also write $\hat{H}|k\rangle = \frac{\hbar^2}{2m}k^2|k\rangle = \frac{Dk^2}{2}|k\rangle$

$$W(x,T \mid x_0,0) = \langle x|e^{-TH}|x_0\rangle = \int dk \int dk' \langle x \mid k'\rangle \langle k'| e^{-TH}|k\rangle\langle k \mid x_0\rangle = \\ = \frac{1}{2\pi}\int dk e^{-\frac{D}{2}Tk^2} e^{ik(x-x_0)} = \frac{1}{\sqrt{2\pi DT}} e^{-\frac{(x-x_0)^2}{2DT}} \quad \langle x \mid k'\rangle = \frac{1}{\sqrt{2\pi}} e^{ik'x} \tag{0.269}$$

This can be generalized to the case of $\hat{H} = -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2} + V(x)$ (Schulman, Ch.9). Similar connections to statistical mechanics as $T \to \beta$ (Ch. 26).

Two-point correlation function (exercise)

With the help of eq. (16) it is easy to calculate the 2-point correlation function which is defined as $\langle x(t_1)\, x(t_2)\rangle$ for $t_0 < t_1 < t_2$. We assume that the particle starts at $x_0 = x(t_0)$.



Average over Brownian trajectories, all starting at x_0 at time $t = t_0$, when looking at the trajectories at times $t = t_1$ and $t = t_2$.

$$\langle x(t_1)\, x(t_2)\rangle_w = \iint d\mathbb{P}_{t_1t_2}(x_1,x_2 \mid x_0,t_0)\, x_1x_2 \tag{0.270}$$

$$= \int_{-\infty}^{+\infty} dx_2 \int_{-\infty}^{+\infty} dx_1 \frac{1}{\sqrt{2\pi D(t_2-t_1)}} e^{-\frac{1}{2D}\frac{(x_2-x_1)^2}{t_2-t_1}} \frac{1}{\sqrt{2\pi D(t_1-t_0)}} e^{-\frac{1}{2D}\frac{(x_1-x_0)^2}{t_1-t_0}} x_2x_1 \tag{0.271}$$

We change variables: $x = x_1 - x_0, y = x_2 - x_1$

$$x_2 = x_0 + x + y \quad x_1 = x + x_0 \quad (x_0 \text{ is a const. }) \tag{0.272}$$

Remember the Jacobian in the transformation:

$$p(x_1,x_2)\, dx_1dx_2 = p\left(x_1(x,y), x_2(x,y)\right)|J|dxdy \tag{0.273}$$

$$J = \begin{pmatrix} \frac{\partial x_1}{\partial x} & \frac{\partial x_1}{\partial y} \\ \frac{\partial x_2}{\partial x} & \frac{\partial x_2}{\partial y} \end{pmatrix} = \begin{pmatrix} 1 & 0 \\ 1 & 1 \end{pmatrix} \Rightarrow |J| = 1 \tag{0.274}$$

From eq. (18) we get

$$\begin{aligned}
&= \int_{-\infty}^{+\infty} dx \int_{-\infty}^{+\infty} dy \frac{1}{\sqrt{2\pi D\left(t_2-t_1\right)}} e^{-\frac{1}{2D}\frac{y^2}{t_2-t_1}} \frac{1}{\sqrt{2\pi D\left(t_1-t_0\right)}} e^{-\frac{1}{2D}\frac{x^2}{t_1-t_0}} \left(x_0+x+y\right)\left(x+x_0\right) \\
&= \int_{-\infty}^{+\infty} dx \frac{e^{-\frac{x^2}{2D\left(t_1-t_0\right)}}}{\sqrt{2\pi D\left(t_1-t_0\right)}} \left(x^2+x_0^2\right) \\
&= D\left(t_1-t_0\right)+x_0^2
\end{aligned} \tag{0.275}$$

Thus for a generic pair of times $t_1, t_2 > t_0$:

$$\left\langle x\left(t_1\right) x\left(t_2\right)\right\rangle_w = D \min\left\{t_1-t_0, t_2-t_0\right\} + x_0^2 \tag{0.276}$$

Exercise: calculate $\left\langle x\left(t_1\right) x\left(t_2\right)\right\rangle_w$ for a generic initial distribution $g\left(x_0\right)$.

Averaging a functional with the Wiener path integral

Functionals of trajectories (say, position of a particle in time) occur many times in Physics. For example, one may want to calculate the average of $F\left(\int_0^T a(s)x(s)ds\right)$, where $x(s)$ is the value of the Brownian trajectory at time s, $a(s)$ is a smooth function of time and F is another smooth function.

For any specific calculation we will rely on the discrete, finite n, formula in eq. (16). Namely, if we wish to find the expected value of a functional such as $F\left(\int_0^T a(t)x(t)dt\right)$, we first take its discrete version, $\sum_i \Delta t_i a\left(t_i\right) x\left(t_i\right)$, use eq. (16) for the calculations and only at the end we take the limit $n \to \infty, \Delta t \to 0$.

In the following we will also use the function $A(s) = \int_s^T a(\tau)d\tau$ which satisfies $\dot{A}(s) = -a(s)$ and $A(T) = 0$. Now, $x(0) = 0$

$$\int_0^T a(s)x(s)ds = -x(s)\int_s^T a(\tau)d\tau\Big|_{s=0}^{s=T} + \int_0^T \dot{x}(s)\left(\int_s^T a(\tau)d\tau\right)ds = \int_0^T \dot{x}(s)A(s)ds \tag{0.277}$$

This can be written down in the discrete form as

$$\int_0^T A(s)\dot{x}(s)ds = \int_0^{x(T)} A(s(x))dx = \lim_{\substack{n\to\infty \\ \max_i(\Delta x_i)\to 0}} \sum_{i=1}^{n} A_i \underbrace{\left(x_i - x_{i-1}\right)}_{\equiv \Delta x_i} \tag{0.278}$$

From now on we set $2D = 1$ (in the end we replace $t \to 2Dt$). We use the Wiener measure in eq. (16) and calculate the average of the discretized functional $F, \langle I_n \rangle$, for a fixed n:

$$\langle I_n \rangle = \int_{\mathbb{R}^n} \prod_{i=1}^{n} \frac{dx_i}{\sqrt{\pi \Delta t_i}} F\left(\sum_{i=1}^{n} A_i \Delta x_i\right) e^{-\sum_{i=1}^{n} \frac{\left(\Delta x_i\right)^2}{\Delta t_i}} \tag{0.279}$$

Now we change variables: $y_i = \Delta x_i$, so $x_i = \sum_{k=1}^{i} y_k + x_0$ for $i = 1, 2 \ldots, n$

Remember: $q(\{y\}) = p(\{x(y)\})\left|\frac{\partial x}{\partial y}\right|$

We have to be careful about the jacobian J:

$$J = \begin{pmatrix} \frac{\partial x_1}{\partial y_1} & \frac{\partial x_1}{\partial y_2} & \cdots & \frac{\partial x_1}{\partial y_n} \\ \vdots & \vdots & \ddots & \vdots \\ \frac{\partial x_n}{\partial y_1} & \frac{\partial x_n}{\partial y_2} & \cdots & \frac{\partial x_n}{\partial y_n} \end{pmatrix} = \begin{pmatrix} 1 & 0 & \cdots & 0 \\ 1 & 1 & \cdots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 1 & 1 & \cdots & 1 \end{pmatrix} \Rightarrow \det J = 1 \quad (0.280)$$

hence

$$\langle I_n \rangle = \int_{\mathbb{R}^n} \prod_{i=1}^{n} \frac{dy_i}{\sqrt{\pi \Delta t_i}} F\left(\sum_i A_i y_i \right) e^{-\sum_i \frac{y_i^2}{\Delta t_i}} \quad (0.281)$$

Now we use a little trick. As $\delta(z) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} e^{ikz} dk$ and $F\left(\sum_i A_i y_i\right) = \int F(z) \delta\left(z - \sum_i A_i y_i\right) dz$, we can write eq. (21) as

$$\begin{aligned} \langle I_n \rangle &= \int \prod_i \frac{dy_i}{\sqrt{\pi \Delta t_i}} \int \frac{dk dz}{2\pi} F(z) e^{ik\left(z - \sum_j A_j y_j\right)} e^{-\sum_i \frac{y_i^2}{\Delta t_i}} \\ &= \int_{-\infty}^{+\infty} \frac{dk dz}{2\pi} e^{ikz} F(z) \int_{\mathbb{R}^n} \prod_i \frac{dy_i}{\sqrt{\pi \Delta t_i}} e^{-\sum_j \left(\frac{y_j^2}{\Delta t_j} + i A_j y_j k \right)} \\ &= \int_{-\infty}^{+\infty} \frac{dk dz}{2\pi} e^{ikz} F(z) e^{-\frac{k^2}{4} \sum_i A_i^2 \Delta t_i} = \int dz F(z) \int \frac{dk}{2\pi} e^{-\frac{k^2}{4} \sum_i A_i^2 \Delta t_i + ikz} \\ &= \int dz F(z) \frac{e^{-\frac{z^2}{\sum_i A_i^2 \Delta t_i}}}{\left(\pi \sum_i A_i^2 \Delta t_i\right)^{1/2}} = \int_{-\infty}^{+\infty} dz F(z) N_z\left(0, \frac{1}{2} \sum_i A_i^2 \Delta t_i\right) \end{aligned} \quad (0.282)$$

Hence

$$\left\langle F\left(\sum_i A_i \Delta x_i \right) \right\rangle_{BM} = \int_{-\infty}^{+\infty} dz F(z) N_z(0, \frac{1}{2} \sum_i A_i^2 \Delta t_i) \quad (0.283)$$

Where $N_z\left(\mu, \sigma^2\right)$ is the Normal distribution with mean μ and variance σ^2. We can now take the limit $n \to \infty, \Delta t_i \to 0$:

$$\sum_i A_i^2 \Delta t_i \longrightarrow \int_0^T A^2(s) ds = \int_0^T \left(\int_s^T a(\tau) d\tau \right)^2 ds \equiv R(T) \quad (0.284)$$

Thus the continuum formulation gives:

$$\left\langle F\left(\int_0^T a(s) x(s) ds \right) \right\rangle_{BM} = \int_{-\infty}^{+\infty} dz F(z) N_z(0, DR(T)) \quad (0.285)$$

where $R(T)$ is defined in (23). If we introduce $2D$, we get

$$N_z(0, 2DR(T)) = \frac{1}{\sqrt{4\pi DR(T)}} e^{-\frac{z^2}{4DR(T)}} \quad (0.286)$$

Example: If $F(z) = e^{hz}$ we obtain the moment generating function of $\int_0^T a(s) x(s) ds$, namely

$$\left\langle e^{h \int_0^T a(s) x(s) ds} \right\rangle_{BM} = e^{DR(T) h^2} \quad (0.287)$$

Exercise: Take $F(z) = e^z$, $a(s) = h_1 \delta(t_1 - s) + h_2 \delta(t_2 - s)$ for $0 < t_1, t_2 <$

T. Calculate $A(s)$ and $R(T)$. Since $\int_0^T a(s)x(s)ds = h_1 x(t_1) + h_2 x(t_2)$, calculate $z(h_1, h_2) = \left\langle e^{h_1 x(t_1) + h_2 x(t_2)} \right\rangle_w$ and finally show that

$$\left.\frac{\partial^2 z}{\partial h_1 \partial h_2}\right|_{h_1=0=h_2} = \langle x(t_1)\, x(t_2)\rangle_{BM} = 2D \min\{t_1, t_2\} \qquad (0.288)$$

A brief summary of what we have done:

We have learnt some properties of the Brownian process:

1. It is the most important continuous stochastic process, which is tightly linked to the diffusion equation. It is a Markov process with continuous paths, but very irregular ones as it is nowhere differentiable.
2. We know how to simulate it.
3. It can be used to define a path integral, an object that is not very well defined but (at least in its discrete form) it can be used to calculate some functionals that are useful in Physics and beyond.

At this point we want to use the Brownian motion to build up new continuous stochastic processes. We will do that by defining stochastic differential equations (SDEs). This needs a lot of care because there are many subtleties with continuous stochastic processes. We will look into the main features. There are many books which develop SDEs rigorously.

Introduction to Stochastic Processes **First Semester**

Lecture 8

Date: 2025-10-17 Profesor: Azaele Sandro

0.8 Introduction to Stochastic Processes

We will present basic results from the theory of stochastic processes. Rigorous definitions and proofs need notions of measure theory that we do not introduce nor assume. therefore, this introduction will necessarily be non-rigorous, with some looseness in the definitions and some inaccuracies in the proofs. There are many books which can give you the mathematical rigor that is necessary for obtaining a full understanding of stochastic processes. These notes, instead, wish to provide enough awareness to make you able to use the tools in applied problems (in physics, biology, finance...).

In the following we will connect the diffusion equation to the most important continuous stochastic process: the Brownian motion (or Wiener Process). This is the basis for building up stochastic differential equations whose solutions have continuous trajectories. These are crucial for defining stochastic models that will be used in several fields of physics.

Useful books:

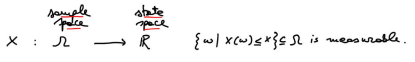
- "Intro. to Stoch. Calculus with Applic.", F.C. Klebaner, Imperial P.
- "An Introd. to SDEs", Lawrence C. Evans, AMS
- "Stoch. Proc. and Applications", G. A. Pavliotis, Springer
- "Stoch. Methods", C. Gardiner, Springer
- "Stoch. Diff. Eq.", B. Oksendal, Springer
- "Stoch. proc. in Physics and chemistry", N.G. van Kampen.

Example: Tossing a coin

Let's assume that we toss a coin 3 times (heads $\to$ 0, tails $\to$ 1) and we ask: what is the sum of the 3 tosses? We define a function from the sample space (the realization) to the state space (what we measure) $Y : \Omega = \{\omega_1 = (0,0,0), \omega_2 = (0,0,1) \dots \omega_8 = (1,1,1)\} \longrightarrow E = \{y_1 = 0, y_2 = 1, y_3 = 2, y_4 = 3\}$ and introduce probabilities $\mathbb{P} : \Omega \to [0,1]$ s.t. $\sum_\omega P(\omega) = 1$; we define $P_i = \sum_{\omega : Y(\omega) = y_i} \mathbb{P}(\omega) = P\left(Y = y_i\right)$. More generally, we can define probabilities for all sets of type $Y^{-1}(B) \subseteq \Omega$, for $B \subseteq E$. This means that Y is a measurable function and this defines a random variable. When Ω is finite, $Y(\Omega)$ is finite and we can always define a random variable as before. We can also define the expectation as

$$E(Y) = \sum_{\omega \in \Omega} Y(\omega)\mathbb{P}(\omega) = \sum_{i=1}^{4} y_i P\left(Y = y_i\right) = \sum_{i=1}^{4} y_i P_i \qquad (0.289)$$

When Ω is an uncountable set, the definition of r.v. needs much care, because we have to make sure that x is still a measurable function. In simple terms x is a real-valued random variable when we can assign probabilities to sets (called events) of the form $\{x \le c\}$ and $\{a < x \le b\}$ for $x, a, b \in \mathbb{R}$.



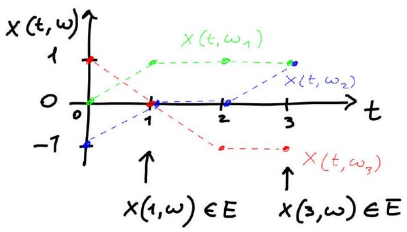
More precisely, a random variable is a measurable function for which the preimage of any Borel set in $\mathbb{R}$ is a measurable set in Ω.

Definition of stochastic process

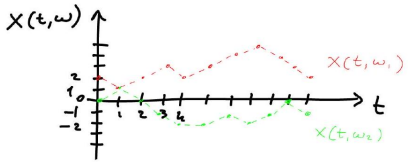
A stochastic process is a collection of random variables $\{x(t,\omega), t \in T, \omega \in \Omega\}$, where T is an ordered set ("time") (it can be either discrete, $T = \mathbb{Z}_+$, or continuous, $T = \mathbb{R}^+$). For each fixed time $t \in T$, $x(t,\omega)$ indicates a random variable from Ω (rigorously, from the probability space $(\Omega, \mathcal{F}, \mathbb{P})$) to E (rigorously, E is a measurable space equipped with a σ-algebra; for instance, $E = \mathbb{R}^d$ and the σ-algebra is the one of Borel sets; we need a "filtration" as well). Ω is the common sample space, E is the state space of the process. For each fixed $\omega \in \Omega$, $x(t,\omega)$ is a function of time t that is called a sample path or a stochastic realization of the process. We will usually omit the ω-dependence, i.e., we write $x(t)$.

Examples:

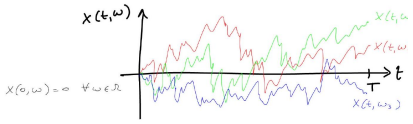
1. Let $E = \{0, 1, -1\}$ be the state space of a stoch-proc x and let $T = \{0, 1, 2, 3\}$ be the (discrete) time. There are then 3^4 sample paths, thus $|\Omega| = 3^4 = 81$.



   In this example we can enumerate all the 81 trajectories. This is not possible if E is an uncountable set.
2. The random walk process in discrete time has $E = \mathbb{Z}$ (position) and $T = \mathbb{N}$ (time), thus $x(t,\omega)$ indicates a stochastic realization (or trajectory) as a function of time t.



   Here we get infinitely countable trajectories ($|\Omega| = |\mathbb{Z}|^{\mathbb{N}}$)
3. The position of a Brownian particle is described by the Brownian process for which $T = \mathbb{R}^+$ and $E = \mathbb{R}$ and one sample path is $x(t,\omega)$



   here every path is a continuous function of time $x(t,\omega) \in C^0([0,T])$

In the following we will omit ω and we will simply write $x(t)$, because what we "observe" is the value $x \in E$ at some time t and not Ω.

Notice that in these examples we have not defined a prob. measure, which is not needed for defining a random variable.

One of the most important stochastic processes is the Brownian process/motion or Wiener process. This can be used to describe the motion of a heavy particle in a fluid made of light particles, which collide with it randomly. For the time being, we will not look into how good this process is for empirical Brownian particles.

Brownian motion (or Wiener process)

A standard Brownian motion in 1-d, $B(t)$, is a real-valued stoch. process ($E = \mathbb{R}, T = \mathbb{R}^+$) for which (A) $B(0) = 0$ (a.s. , namely, Prob. B(0)=0=1) (B) For any $0 \leqslant s < t < \infty, B(t) - B(s)$ is normally distributed, that is $B(t) - B(s) \sim N(0, t-s) = \frac{1}{\sqrt{2\pi(t-s)}} e^{-\frac{\Delta x^2}{2(t-s)}}$ (mean 0 and variance $t - s$) (C) For all times $0 = t_0 < t_1 < t_2 < \ldots < t_n$ the increments $\Delta B_i := B(t_i) - B(t_{i-1})$ are independent (of each other)

Some important properties:

1. Stationarity of increments: notice that, if we write $t = s + \Delta t$, then from (B) we get

$$B(s+ \tag{0.290}$$

$$Deltat) - B(s) \sim N(0, \Delta t) \tag{0.291}$$

   which means that the distribution of $B(s + \Delta t) - B(s)$ does not depend on s. This means that the increments are not only independent, but also stationary, namely they depend only on Δt : $\Delta B = B(s + \Delta t) - B(s) \sim B(\Delta t)$.
   Since $\mathrm{Var}[B(\Delta t)] = \Delta t$, we expect that $|\Delta B| = |B(\Delta t)| \simeq \sqrt{\Delta t}$ as $\Delta t \to 0^+$. This will be crucial in the future, in many calculations.
2. Connection with the diffusion equation
   We have seen that the fundamental solution of the diffusion eq. ($D = 1$)

$$\begin{cases} \partial_t w(x,t) = \dfrac{1}{2}\partial_x^2 w(x,t) & x \in \mathbb{R}, t > t_0 \\ w(x,t_0) = \delta(x - x_0) & t = t_0 \end{cases} \tag{0.292}$$

   is the propagator of the Brownian motion:

$$w(x, t \mid x_0, t_0) = \frac{1}{\sqrt{2\pi(t - t_0)}} e^{-\frac{(x-x_0)^2}{2(t-t_0)}} \tag{0.293}$$

   which is the one we use in (B). So from time to time the process evolves with the propagator (1) and with stationary independent increments.
3. Correlation function
   The average will be indicated either with $\langle \cdots \rangle$ or with $\mathbb{E}(\cdots)$. Let $0 \leqslant s \leqslant t$: from (B) $\mathbb{E}[B(s)] = 0, \mathbb{E}\left[B(s)^2\right] = s$. Then

$$\mathbb{E}[B(t)B(s)] = \mathbb{E}[(B(s) + B(t) - B(s))B(s)] = \quad = \mathbb{E}\left[B(s)^2 + (B(t) - B(s))B(s)\right] = \quad = \mathbb{E}\left[B(s)^2\right] + \mathbb{E}[(B(t) - B(s))B(s)] = \quad = s + \tag{0.294}$$

Thus for $s, t \geqslant 0$

$$\mathbb{E}[B(t)B(s)] = \min(t, s) \tag{0.295}$$

Exercises: i) (Ornstein-Uhlenbeck process). Define $V(t) = e^{-t} B\left(e^{2t}\right)$ where $B(t)$ is a Brownian process. Show that $\mathbb{E}[V(t)] = 0$ and $\mathbb{E}[V(t)V(s)] = e^{-|t-s|}$. ii) (Brownian bridge). Define $V(t) = B(t) - (t/T)B(T)$ for any $t \in [0, T]$, Where $B(t)$ is a Brownian process. Show that $\mathbb{E}[V(t)] = 0$ and $\mathbb{E}[V(t)V(s)] = \min(t, s) - ts/T$ for any $t, s \in [0, T]$. iii) Show that $\mathbb{E}\left[e^{i\lambda B(t)}\right] = e^{-\frac{\lambda^2 t}{2}}$ for $t \geqslant 0$, $B(t)$ B.m. iv) With the help of the Law of large numbers and $B(t) = \sum_{i=1}^{t/\Delta t} \Delta B_i$, show that $\lim_{t\to\infty} \frac{B(t)}{t} = 0$.

4. Rescaling. The process $z(t) = \frac{1}{\sqrt{c}} B(ct)$, $c > 0$, is a Brownian motion that is distributed like $B(t)$, another Brownian motion. (Verify (A), (B) and (C)). Also:

$$\mathbb{E}\left[e^{i\lambda z(t)}\right] = \mathbb{E}\left[e^{i\lambda \frac{1}{\sqrt{c}} B(ct)}\right] = e^{-\frac{\lambda^2}{2c} tc} = e^{-\frac{\lambda^2 t}{2}} = \mathbb{E}\left[e^{i\lambda B(t)}\right] \tag{0.296}$$

5. Inversion. The process $z(t) = tB\left(\frac{1}{t}\right)$ for $t > 0$ and $z(0) = 0$ is distributed like $B(t)$, another B.m.

$$\mathbb{E}\left[e^{i\lambda z(t)}\right] = \mathbb{E}\left[e^{i\lambda t B\left(\frac{1}{t}\right)}\right] = e^{-\frac{\lambda^2}{2} t^2 \cdot \frac{1}{t}} = e^{-\frac{\lambda^2 t}{2}} = \mathbb{E}\left[e^{i\lambda B(t)}\right] \tag{0.297}$$

Notice that $\lim_{t\to\infty} \frac{z(t)}{t} = \lim_{t\to\infty} B\left(\frac{1}{t}\right) = 0$ as in (iv).

6. Time reversal. Define $z(t) = B(T) - B(T-t)$ for any $t \in [0, T]$. Then $Z(t)$ and $B(t)$ have the same distrib.

Properties of the trajectories of the Brownian motion

These are hard to prove rigorously, but somehow easy to guess. Let's consider the ratio $\frac{\Delta B}{(\Delta t)^\alpha}$ where $\Delta t = t_2 - t_1 > 0, \alpha > 0$ and $\Delta B = B(t_2) - B(t_1)$. What happens to this ratio as $\Delta t \to 0^+$? Take some $k \in \mathbb{R}^+$:

$$P\left(\left|\frac{\Delta B}{\Delta t^\alpha}\right| \leqslant k\right) = P\left(|\Delta B| \leqslant k\Delta t^\alpha\right) = \int_{-k(\Delta t)^\alpha}^{k(\Delta t)^\alpha} dx \frac{e^{-\frac{x^2}{2\Delta t}}}{\sqrt{2\pi\Delta t}} = \quad = \frac{2}{\sqrt{2\pi\Delta t}} \int_0^{k(\Delta t)^\alpha} dx e^{-\frac{x^2}{2\Delta t}} = \frac{2}{\sqrt{2\pi}} \int_0^{k(\Delta t)^{\alpha-1/2}} dz e^{-z^2/2} \tag{0.298}$$

Here are the consequences:

1. $0 < \alpha < \frac{1}{2}$, as $\Delta t \to 0^+$, $\quad P\left(\left|\frac{\Delta B}{\Delta t^\alpha}\right| \leqslant k\right) \to 1$ regardless of k. This tells us that as $|t - s| \to 0^+$

$$|B(t) - B(s)| \leqslant \text{ const } |t - s|^\alpha \tag{0.299}$$

which means that Brownian trajectories are Hölder continuous for any $0 < \alpha < \frac{1}{2}$. This can be proven rigorously.

2. $\alpha = 1$ (or $\frac{1}{2} < \alpha \leqslant 1$), as $\Delta t \to 0^+, P\left(\left|\frac{\Delta B}{\Delta t}\right| \leqslant k\right) \to 0 \quad \forall k \in \mathbb{R}^+$

This tells us that the Brownian trajectories are nowhere differentiable. This is expected because if $|\Delta B| \sim \sqrt{Deltat}$, then $\frac{|\Delta B|}{\Delta t} \sim \frac{1}{\sqrt{\Delta t}}$ and hence $\lim_{\Delta t\to 0^+} \frac{|\Delta B|}{\Delta t} \to \infty$. This is related to the fact that B.m. has no memory of the past (see the Markov property below).

We can add a drift
mu and change the diffusion coefficient of a Brownian motion with no difficulty. We define a Brownian motion with drift
mu and variance D the process

$$x(t) = x_0 + \mu t + \sqrt{2D}B(t) \tag{0.300}$$

Verify that $\mathbb{E}[x(t)] = x_0 + \mu t$ and $\mathrm{Var}[x(t)] \equiv \mathbb{E}\left[(x(t) - \mathbb{E}[x(t)])^2\right] = 2Dt$. Notice that $x(t)$ satisfies the stochastic differential equation:

$$dx(t) = \mu dt + \sqrt{2D}dB(t) \tag{0.301}$$

How to simulate a very simple SDE (including B.m.) We wish to generate a path of eq. (5), starting from $x(0) = x_0$. Because $\Delta B \sim B(\Delta t) \sim \sqrt{\Delta t}B(1)$ for finite times $t_0 = 0 < t_1 \cdots < t_{n-1} < t_n$ we can write (5) as ($\Delta t = t_i - t_{i-1}$)

$$\begin{aligned} x(t_i) &= x(t_{i-1}) + \mu\Delta t + \sqrt{2D\Delta t}\varepsilon_i \qquad i = 1, 2, \ldots, n \\ x(0) &= x_0 \end{aligned} \tag{0.302}$$

where $\varepsilon_i \sim N(0, 1)$. Notice that we use a sequence of n independent and identically distributed random variables ε_i drawn from $N(0, 1)$ because at every time step we add a random value that is independent of all values that were calculated before (indep. of $x, t, \mu, D \ldots$). Of course, $\mu = 0, D = 1/2$ and $x_0 = 0$ generate a standard Brownian motion as defined in (A), (B) and (C).

Markov processes

Let us focus on a stochastic process for which we can take a set of ordered times, i.e. $t_0 < t_1 < t_2 \cdots < t_n$ and there exists a conditional prob. density funct. at time t_n, namely $p_{1|n-1}(x_n, t_n \mid x_{n-1}, t_{n-1}; \ldots; x_1, t_1; x_0, t_0)$. This PDF tells us what is the prob. of observing x_n at time t_n, if we know what happened to the process at previous times; we really know the actual values that occurred, not only their probabilities. This is quite a lot of information and basically it means that, if we want to make a prediction on what is going to happen in the future, we have to know all that happened in the past. However, in some situations the effect of the past can be neglected. In particular, if it happens that for any $n = 1, 2 \ldots$

$$p_{1|n-1}(x_n, t_n \mid x_{n-1}, t_{n-1}; \ldots; x_1, t_1; x_0, t_0) = p_{1|1}(x_n, t_n \mid x_{n-1}, t_{n-1}) \tag{0.303}$$

Then we say that the stochastic process is a Markov process. This means that predictions at time t_n only depend on what happened at time t_{n-1} and not on the whole history of the process. The pdf $p_{1|1}$ is called transition probability or propagator.

A Markov process can be fully defined by two functions: the propagator $p_{1|1}$ and the initial distribution $p_1(x_0, t_0)$.

Indeed the 3-point joint PDF for a Markov process is ($t_0 < t_1 < t_2$):

$$\begin{aligned} P_3(x_2t_2; x_1t_1; x_0t_0) &= P_{1|2}(x_2t_2 \mid x_1t_1; x_0t_0)\, P_2(x_1t_1; x_0t_0) = \qquad = p_{1|1}(x_2t_2 \mid x_1t_1)\, P_2(x_1t_1; x_0t_0) \\ &= P_{1|1}(x_2t_2 \mid x_1t_1)\, P_{1|1}(x_1t_1 \mid x_0t_0)\, P_1(x_0t_0) \end{aligned} \tag{0.304}$$

Therefore we can find iteratively

$$p_n(x_n t_n; x_{n-1} t_{n-1}; \ldots; x_1 t_1; x_0 t_0) = \prod_{i=1}^{n} p_{1|1}(x_i t_i \mid x_{i-1} t_{i-1})\, p_1(x_0 t_0) \quad (0.305)$$

this property makes Markov processes much more amenable to analytical calculations than non-Markov ones.

The Chapman-Kolmogorov equation

Not all functions can be used as propagators for Markov processes, nor an initial distribution p_1 can be arbitrary. These two functions must satisfy two identities, one of which is the C-K. equation.

From the L.H.S. of eq. (8), if we integrate wrt x_1,

$$\int dx_1 p_3(x_2 t_2; x_1 t_1; x_0 t_0) = p_2(x_2 t_2; x_0 t_0) \quad (0.306)$$

from the R.H.S., instead

$$= \int dx_1 p_{1|1}(x_2 t_2 \mid x_1 t_1)\, p_{1|1}(x_1 t_1 \mid x_0 t_0)\, p_1(x_0 t_0) \quad (0.307)$$

but $p_2(x_2 t_2; x_0 t_0) = p_{1|1}(x_2 t_2 \mid x_0 t_0)\, p_1(x_0 t_0)$, because of the Markov property, so

$$p_{1|1}(x_2 t_2 \mid x_0 t_0)\, p_1(x_0 t_0) = \int dx_1 p_{1|1}(x_2 t_2 \mid x_1 t_1)\, p_{1|1}(x_1 t_1 \mid x_0 t_0)\, p_1(x_0 t_0) \quad (0.308)$$

hence, for any $t_2 > t_1 > t_0$

$$p_{1|1}(x_2 t_2 \mid x_0 t_0) = \int dx_1 p_{1|1}(x_2 t_2 \mid x_1 t_1)\, p_{1|1}(x_1 t_1 \mid x_0 t_0) \quad (0.309)$$

this is the Chapman-Kolmogorov equation (actually, identity), which must be satisfied by any propagator/transition probab. If we further integrate eq. (10) w.r.t. x_0 we get

$$\int dx_0 p_{1|1}(x_2 t_2 \mid x_0 t_0)\, p_1(x_0 t_0) = p_1(x_2 t_2) \quad (0.310)$$

and

$$\int dx_0 p_{1|1}(x_1 t_1 \mid x_0 t_0)\, p_1(x_0 t_0) = p_1(x_1 t_1) \quad (0.311)$$

we obtain, for $t_2 > t_1$,

$$p_1(x_2 t_2) = \int dx_1 p_{1|1}(x_2 t_2 \mid x_1 t_1)\, p_1(x_1 t_1) \quad (0.312)$$

this is the 2$^{\text{nd}}$ eq. (identity) for a Markov process. Therefore p_1 and $p_{1|1}$ are connected to each other. It can be proven that any two non-negative functions that satisfy eqs. (11) and (12) define a Markov process.

Stationary Markov Process

If p_1 is independent of time and equal to the equilibrium distribution of the stochastic process, and $p_{1|1}$ depends only on the time difference $left|t_2 - t_1 ight|$, then the process is a stationary Markov process.

The Brownian motion is a Markov process This property essentially follows from the independence of the increments and it can be proven in different ways. In our context, we can use eq. (1), i.e. the propagator

$$P_{1|1}\left(x_1, t_1 \mid x_0, t_0\right) \equiv W\left(x_1, t_1 \mid x_0, t_0\right) = \frac{1}{\sqrt{2\pi D\left(t_1 - t_0\right)}} e^{-\frac{\left(x_1 - x_0\right)^2}{2D(t_1 - t_0)}} \quad (0.313)$$

and show that eq. (11) is satisfied by direct integration. Also, if you take $P_1\left(y_1, t_1 = 0\right) = \delta\left(y_1\right)$ you get from eq. (12) $p_1\left(y_2, t_2\right) = \frac{1}{\sqrt{2\pi D t_2}} e^{-y_2^2/2Dt_2}$. These generate a non-stationary Markov process.

Exercises:

1. Show that the Poisson process defined by

$$P_{1|1}\left(x_2 t_2 \mid x_1 t_1\right) = \frac{\left(\lambda\left(t_2 - t_1\right)\right)^{x_2 - x_1}}{\left(x_2 - x_1\right)} e^{-\lambda(t_2 - t_1)} \quad t_2 > t_1 \quad (0.314)$$

   and $P_1(n, 0) = \delta_{n,0} \Rightarrow P_1(n, t) = \frac{(\lambda t)^n}{n!} e^{-\lambda t}$ is a (non-stationary) Markov process.
2. Show that for $x, y = \pm 1$ the function

$$P_{1|1}\left(xt \mid yt'\right) = \frac{1}{2}\left[1 + e^{-2\gamma(t - t')}\right]\delta_{xy} + \frac{1}{2}\left[1 - e^{-2\gamma(t - t')}\right]\delta_{x,-y} \quad (0.315)$$

   satisfies eq. (11).
3. Show that the process defined by

$$P_1(x) = \frac{1}{\sqrt{2\pi}} e^{-x^2/2} \quad (0.316)$$

   $p_{1|1}\left(xt \mid y, t'\right) = \frac{1}{\sqrt{2\pi\left(1 - e^{-2|t - t'|}\right)}} \exp\left[-\frac{\left(x - ye^{-|t - t'|}\right)^2}{2\left(1 - e^{-2|t - t'|}\right)}\right]$ is a stationary Markov process. This is called the O.U. proc.

Wick's theorem **First Semester**

Lecture 9

Date: 2025-10-17 Profesor: Azaele Sandro

0.9 Wick's theorem

Note that, because of symmetry, the s-point correlation for s any odd integer is zero (the Gaussian remains unchanged if $\vec{x} \to -\vec{x}$).

What happens when we want to calculate $\langle x_i x_j \cdots x_l \rangle$? Should we always do all the derivatives as in eq. (12)? No! If the vars are Gaussian we can use

Wick's theorem

Any correlation between an even number of Gaussian r.v. can be written down as a sum of products of 2-point correlation functions $\left(A^{-1}\right)$. For instance

$$\begin{gathered}\langle x_a x_b x_c x_d \rangle = \langle x_a x_b \rangle \langle x_c x_d \rangle + \langle x_a x_c \rangle \langle x_b x_d \rangle + \langle x_a x_d \rangle \langle x_b x_c \rangle \\ \left(A^{-1}\right)_{ab} \quad \left(A^{-1}\right)_{cd} \quad \cdots \quad \text{(indexes may be equal)}\end{gathered} \tag{0.317}$$

Exercise: from the previous case, show that (no calculations!)

$$\begin{aligned}\left\langle x_1^2 x_2^2 \right\rangle &= \langle x_1 x_1 \rangle \langle x_2 x_2 \rangle + 2 \langle x_1 x_2 \rangle^2 = \frac{3}{8} \cdot \frac{3}{8} + 2 \left(\frac{1}{8}\right)^2 = \frac{11}{64} \\ \left\langle x_1^4 \right\rangle &= 3 \left\langle x_1^2 \right\rangle^2 = 3 \left(\frac{3}{8}\right)^2 = \frac{27}{64}\end{aligned} \tag{0.318}$$

In general:

$$\underbrace{\langle x_i x_j \ldots x_n x_m \rangle}_{s \text{ vars}} = \sum_p \left(A^{-1}\right)_{i_p j_p} \cdots \left(A^{-1}\right)_{n_p m_p} \tag{0.319}$$

Where the sum runs over all pairings of s indexes, i.e. over all ways of grouping s (even) indexes $i, j \ldots, n, m$ into pairs (counting the pair even when indexes are equal; order in the pairs is not important). If there are s vars then the possible pairings are $(s-1)!! = (s-1)(s-3)\ldots 3 \cdot 1$.

Further important results obtained with characteristic functions

(1) If you are given two independent and identically distributed (iid) random variables, how do you calculate the pdf of their sum? What is its c.f.? We assume they are real with pdf $q(x)$:

$$x = x_1 + x_2 \quad x_1, x_2 \sim q(x) \tag{0.320}$$

When we draw x_1 and x_2 from $q(x)$, many different outcomes can give you the same sum x, these have to be added up with the corresponding probability, hence

$$p(x) = \int \delta\left(x - (x_1 + x_2)\right) p\left(x_1, x_2\right) dx_1 dx_2 \equiv \langle \delta\left(x - x_1 - x_2\right) \rangle \tag{0.321}$$

we select all possible x_1, x_2 s.t. their sum is x. i.i.d.

$$\begin{aligned} &= \int \delta\left(x - x_1 - x_2\right) q\left(x_1\right) q\left(x_2\right) dx_1 dx_2 \\ &= \int q(x-y) q(y) dy \quad \text{it's a convolution.} \end{aligned} \tag{0.322}$$

What is the c.f. of $p(x)$ if the c.f. of $q(x)$ is $\varphi_1(k)$?

$$\varphi(k) \equiv \left\langle e^{ikx} \right\rangle = \int e^{ikx} p(x) dx = \int dx e^{ikx} \delta\left(x - (x_1 + x_2)\right) q\left(x_1\right) q\left(x_2\right) dx_1 dx_2 \tag{0.323}$$
$$= \int e^{ik(x_1+x_2)} q\left(x_1\right) q\left(x_2\right) dx_1 dx_2 = \left[\varphi_1(k)\right]^2$$

What happens if the r.v. are independent but not identically distributed? (2) The (weak) law of large numbers (convergence in distribution) If we are now given n iid r.v. whose pdf is $q(x)$ with c.f. $\varphi_1(k)$, what happens to $X = \frac{1}{n}\sum_i x_i$ as $n \to \infty$? Let's assume that the mean of x_i is $\mu \quad \left(\mu = \int x q(x) dx < \infty\right)$. (See Grimmett Stirzaker, p. 193, Prob. and Random Processes). proof: Let $\varphi_n(k)$ be the c.f. of the average of the rand. variables

$$\varphi_n(k) \equiv \left\langle e^{ikX} \right\rangle = \left\langle e^{ik\frac{1}{n}\sum_i x_i} \right\rangle = \int e^{\frac{ik}{n}\sum_i x_i} q\left(x_1\right) \cdots q\left(x_n\right) dx_1 \cdots dx_n \tag{0.324}$$

$$= \left(\int e^{i\frac{k}{n}x_1} q\left(x_1\right) dx_1\right) \cdots \left(\int e^{ik\frac{x_n}{n}} q\left(x_n\right) dx_n\right) = \left(\varphi_1\left(\frac{k}{n}\right)\right)^n \tag{0.325}$$

Also, Taylor

$$\varphi_1\left(\frac{k}{n}\right) = 1 + \frac{ik}{n}\langle x \rangle + O\left(\frac{1}{n^2}\right) \text{ as } n \to \infty \tag{0.326}$$

From (17)

$$\left(1 + \frac{ik}{n}\langle x \rangle + \ldots\right)^n \xrightarrow[n\to\infty]{} e^{i\mu k} = \int \delta(x-\mu) e^{ikx} dx \tag{0.327}$$

Here we have only proved that we have a much stronger result:

$$\frac{1}{n}\sum_{i=1}^{n} x_i \to \mu \tag{0.328}$$

The strong law of large numbers states: Let $x_1 \ldots x_n$ be a sequence of i.i.d. r.v. each with finite mean μ. Then the finite (empirical) average approaches μ as $n \to \infty$. (Grimmett, p. 329) This law tells us that, for large n, the sum $\sum_i x_i$ is approximately $n\mu$. Of course there will be fluctuations around $n\mu$. A natural question is then what can we say about $\sum_{i=1}^n x_i - \mu n$? There is an extraordinary answer to this question, which is valid whenever x_i have finite variance: a) $\sum_{i=1}^n x_i - \mu n$ is about as big as $\sqrt{n}$ b) The distribution of $\frac{\sum_{i=1}^n x_i - \mu n}{\sqrt{n}}$ approaches a Gaussian pdf as $n \to \infty$ IRRESPECTIVE of the pdf of x_i.

Claims a) and b) are the core meaning of the

Central Limit Theorem

Let $x_1 \dots x_n$ be a sequence of i.i.d. r.v. with finite mean μ and finite (non-zero) variance σ^2. Then the p.d.f. of

$$Y_n = \frac{\sum_{i=1}^{n} x_i - \mu n}{\sqrt{n}\sigma} \xrightarrow[n\to\infty]{\text{conv. in distrib.}} N(0,1) \tag{0.329}$$

Obs: $\langle Y_n \rangle = \frac{1}{\sqrt{n}\sigma} \left(\sum_i \langle x_i \rangle - \mu n \right) = 0$

$$\mathrm{Var}\,(Y_n) = \frac{1}{n\sigma^2} \mathrm{Var} \left(\sum_{i=1}^{n} x_i - \mu n \right) = \frac{1}{n\sigma^2} \mathrm{Var} \left(\sum_{i=1}^{n} x_i \right) = \frac{\sum_i \mathrm{Var}\,(x_i)}{n\sigma^2} = \frac{n\sigma^2}{n\sigma^2} = 1 \tag{0.330}$$

(please, go throughly 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. proof: Let's assume that each r.v. has a p.d.f. $q(x)$ with c.f. $\varphi_1(k)$, $\varphi_n(k)$ is the c.f. of Y_n:

$$\varphi_n(k) = \left\langle e^{ikY_n} \right\rangle = \int e^{ik \frac{\sum_i x_i - \mu n}{\sqrt{n}\sigma}} q\,(x_1) \cdots q\,(x_n)\, dx_1 \cdots dx_n = \tag{0.331}$$

$$= e^{-\frac{ik\mu\sqrt{n}}{\sigma}} \left(\int e^{\frac{ikx}{\sqrt{n}\sigma}} q(x) dx \right)^n = e^{-\frac{ik\mu\sqrt{n}}{\sigma}} \left(\varphi_1 \left(\frac{k}{\sqrt{n}\sigma} \right) \right)^n \tag{0.332}$$

As in the previous theorem we can expand φ_1 as $n \to \infty$

$$\varphi_1 \left(\frac{k}{\sqrt{n}\sigma} \right) = 1 + \frac{ik}{\sqrt{n}\sigma} \langle x \rangle - \frac{k^2}{2n\sigma^2} \left\langle x^2 \right\rangle + O\left(n^{-3/2} \right) = e^{\frac{ik\mu}{\sqrt{n}\sigma} - \frac{k^2}{2n}} \tag{0.333}$$

from (20)

$$\varphi_n(k) = e^{-\frac{ik\mu}{\sigma}\sqrt{n}} e^{\frac{ik\mu}{\sigma}\sqrt{n} - \frac{k^2}{2}} = e^{-\frac{k^2}{2}} \tag{0.334}$$

As we have shown in eq. (6), this is the c.f. of $p(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \equiv N(0,1)$. Show 1) $\sum_{i=1}^{n} x_i \sim N\left(n\mu, n\sigma^2\right)$; 2) $\frac{1}{n} \sum_{i=1}^{n} x_i \sim N\left(\mu, \frac{\sigma^2}{n}\right)$

Introduction to Stochastic Differential Equations **First Semester**

Lecture 10

Date: 2025-10-17 Profesor: Azaele Sandro

0.10 Introduction to Stochastic Differential Equations

We have already seen a very simple example of SDE in eq. (4) and (5) where $x(t) = x_0 + \mu t + \sigma B(t)$ or $dx = \mu dt + \sigma dB(t)$. This was also easy to integrate numerically. Usually an ODE has the form

$$\frac{dx}{dt} = f(x,t) \tag{0.335}$$

Can we write an SDE in this usual form? Let's try. We get from

$$\frac{dx}{dt} = \mu + \sigma \dot{B}(t) \tag{0.336}$$

What is $\dot{B}$? Actually it does not exist because we have seen that Brownian motion is nowhere differentiable. However, $\Delta B = B(t+\Delta t) - B(t)$ is well defined, so mathematicians prefer the notation $dx = \mu dt + \sigma dB$. However, we can give a meaning to the "pseudo notation" $\dot{B}$. We first discretize and then take the limit as $\Delta t \to 0$; so we define for a finite $\Delta t \quad \xi_{\Delta,i} = \frac{\Delta B_i}{\Delta t}, \Delta B_i \equiv B(t_i + \Delta t) - B(t_i)$. As we know, ΔB_i does not depend on t_i, but this notation is useful in the following. Of course, $\langle \xi_{\Delta,i} \rangle = 0$. In order to understand what $\left\langle \xi_{\Delta,i} \xi_{\Delta,j} \right\rangle$ is, let's take a test function $g(t)$ and calculate at $g_i \equiv g(t_i)$ the following

$$\sum_j g_j \left\langle \xi_{\Delta,i} \xi_{\Delta,j} \right\rangle \Delta t = \sum_j g_j \left\langle \frac{\Delta B_i}{\Delta t} \frac{\Delta B_j}{\Delta t} \right\rangle \Delta t = \sum_j g_j \frac{\left\langle \Delta B_i \Delta B_j \right\rangle}{\Delta t} = \sum_j g_j \frac{\delta_{ij} \Delta t}{\Delta t} = g_i \tag{0.337}$$

N.B: $\left\langle \Delta B_i \Delta B_j \right\rangle = \delta_{ij} \Delta t$

If we now take the continuum limit $\Delta t \to 0$, and "$\lim_{\Delta t \to 0} \xi_{\Delta,i} \equiv \xi(t)$" we get

$$\int g(t') \langle \xi(t) \xi(t') \rangle \, dt' = g(t) \tag{0.338}$$

Which therefore means that $\langle \xi(t) \xi(t') \rangle = \delta(t - t')$ and $\langle \xi(t) \rangle = 0$. This is called Gaussian white (or δ-correlated) noise; with this we can then write the SDE in eq. (4) as

$$\begin{array}{l} \dot{x}(t) = \mu + \sigma \xi(t) \\ \langle \xi \rangle = 0 \quad \langle \xi(t) \xi(t') \rangle = \delta(t - t') \end{array} \quad \text{is equivalent to} \quad dx = \mu dt + \sigma dB \tag{0.339}$$

$B(t)$ is a standard B.M. $\langle B(t) \rangle = 0, \langle B(t) B(s) \rangle = t \wedge s$

The first one is a notation which physicists like the most, whereas mathematicians prefer $dx = \mu dt + dB$, you can find both in the literature.

What is a solution?

If we start from a deterministic eq like

$$dx = f(x,t) dt \tag{0.340}$$

there are many ways to introduce noise. We could define a stoch. process by saying that $dx = \tilde{f}(x, t, dB)dt$ where $\tilde{f}$ is a generic non-linear smooth function. However this definition does not work in general and it is very difficult to define appropriately what that exactly means and to able to find solutions. The approach that works in many situations, even in higher dimensions under general assumptions is to introduce the noise (better, Brownian motion) in an additive way. This means that we can develop a good deal of theory for SDEs of the form

$$dx = \mu(x, t)dt + \sigma dB(t) \quad (\sigma > 0) \tag{0.341}$$

where μ is a smooth function of x, t. This eq. can be also justified on physical grounds as we will see in the following (if $x(t)$ is the position of a large particle in a fluid, σdB can represent the effect of all other small fluid particles at temperature T, and $\sigma = \sigma(T)$, which continuously kick the large one. All kicks produce the erratic movement of the big suspended particle). Eq. (27) is called Langevin equation with additive noise. However, even simple equations such as this one

$$dx = -\mu x dt + \sigma dB \tag{0.342}$$

can hide pitfalls. For instance, $\langle dx \rangle = -\mu \langle x \rangle dt$, so $\frac{d\langle x \rangle}{dt} = -\mu \langle x \rangle$ hence $\langle x(t) \rangle = x_0 e^{-\mu t}$. But what about fluctuations?

We need to calculate $\left\langle x^2 \right\rangle$. Let's proceed naively with ordinary calculus: $\frac{dx^2}{dt} = 2x\frac{dx}{dt}$, so $2xdx = -2\mu x^2 dt + 2\sigma x dB$ and $d\left\langle x^2 \right\rangle = 2\langle x dx \rangle = -2\mu \left\langle x^2 \right\rangle dt + 2\sigma \langle x dB \rangle = -2\mu \left\langle x^2 \right\rangle dt$ then $\frac{d\left\langle x^2 \right\rangle}{dt} = -2\mu \left\langle x^2 \right\rangle \Rightarrow \left\langle x^2 \right\rangle = x_0^2 e^{-2\mu t}$. But then

$$\sqrt{\langle x^2 \rangle} = x_0 e^{-\mu t} = \langle x \rangle \Rightarrow \mathrm{Var}[x(t)] = 0! \tag{0.343}$$

So there are no fluctuations even if we add the noise! Either ordinary calculus cannot be used or $\langle x dB \rangle \neq 0$. This is a consequence of the non-differentiability of B.

We can consider SDEs even more general SDEs than eq.(27) driven by Brownian motion

$$dx = \mu(x, t)dt + \sigma(x, t)dB \tag{0.344}$$

This is an SDE with multiplicative noise because σ is a function of the state x. Eq. (28) needs extra care!

If we have a (strong) solution $x(t)$ of eq. (28) then we can write

$$x(t) = x(0) + \int_0^t \mu(x(s), s)ds + \int_0^t \sigma(x(s), s)dB(s) \tag{0.345}$$

A strong solution is some functional $F(t, B(s), s \leq t)$ of the Brownian motion $B(t)$. This becomes the solution of the corresponding ODE as $\sigma = 0$.

Warning: What is the meaning of $\int_0^t \sigma(x(s), s)dB(s)$? Can this be understood as an ordinary integral? No.

Let's take a very simple example. If the process is simply ($\mu = 0$ and

$\sigma = B$):

$$dx = B(t)dB(t) \tag{0.346}$$

the solution is $X(t) = \int_0^t B(s)dB(s)$ So we naively expect $E[x(t)] = 0$

If we use ordinary calculus then

$$x(t) = \frac{B(t)^2}{2} \tag{0.347}$$

but then $\mathbb{E}[x(t)] = \frac{t}{2} \neq 0$. What's going on here? Again, because Brownian motion is very irregular, it gives rise to problems where interpreting solutions or eqs.

Before showing what the nature of the problem is, we have to prove an important property of the Brownian m.

LEMMA: The Brownian motion has finite quadratic variation

Let's fix $t > 0$, take the interval $[0, t]$ and partitions $\mathcal{P}_n$ of the interval $\{t_0 = 0 < t_1 < t_2 \cdots < t_n = t\}$ such that $|\mathcal{P}_n| \equiv \max_i |t_i - t_{i-1}| \to 0$ as $n \to \infty$. Then

$$\text{ms-lim}_{\substack{n\to\infty \\ |\mathcal{P}_n|\to 0}} \sum_{i=0}^{n-1} \underbrace{\left[B\left(t_{i+1}\right) - B\left(t_i\right)\right]^2}_{\text{quadratic variation}} = t \tag{0.348}$$

Reminder: $ms - \lim_{n\to\infty} x_n = x$ means $\lim_{n\to\infty} \left\langle \left(x_n - xight\right)^2 \right\rangle = 0$ this is the mean square limit and we say that x_n converges to x in the mean square.

Proof: Let's define $Q_n \equiv \sum_{i=0}^{n-1} \left[B\left(t_{i+1}\right) - B\left(t_i\right)\right]^2$ and take

$$Q_n - t = \sum_i \left\{\left[B\left(t_{i+1}\right) - B\left(t_i\right)\right]^2 - \left(t_{i+1} - t_i\right)\right\} \tag{0.349}$$

Hence we have to evaluate as $n \to \infty \quad \left(B\left(t_i\right) \equiv B_i\right)$

$$\mathbb{E}\left[\left(Q_n - t\right)^2\right] = \sum_{i=0}^{n-1}\sum_{j=0}^{n-1} \mathbb{E}\left[\left\{\left(B_{i+1} - B_i\right)^2 - \left(t_{i+1} - t_i\right)\right\}\left\{\left(B_{j+1} - B_j\right)^2 - \left(t_{j+1} - t_j\right)\right\}\right] \tag{0.350}$$

For $i \neq j$

$$\begin{aligned} &\mathbb{E}\left[\left\{\left(B_{i+1} - B_i\right)^2 - \left(t_{i+1} - t_i\right)\right\}\left\{\left(B_{j+1} - B_j\right)^2 - \left(t_{j+1} - t_j\right)\right\}\right] \\ &= \mathbb{E}\left[\left\{\left(B_{i+1} - B_i\right)^2 - \left(t_{i+1} - t_i\right)\right\}\right] \mathbb{E}\left[\left\{\left(B_{j+1} - B_j\right)^2 - \left(t_{j+1} - t_j\right)\right\}\right] = 0 \end{aligned} \tag{0.351}$$

$\mathbb{E}\left[\left(B_{i+1} - B_i\right)^2\right] = t_{i+1} - t_i$

Therefore eq. (29b) becomes

$$\begin{aligned}\mathbb{E}\left[(Q_n - tight)^2\right] &= \sum_{i=0}^{n-1} \mathbb{E}\left[\left\{(B_{i+1}-B_i)^2 - (t_{i+1}-t_i)\right\}^2\right] \\ &= \sum_i \left\{\mathbb{E}\left[(B_{i+1}-B_i)^4\right] - 2\mathbb{E}\left[(B_{i+1}-B_i)^2\right](t_{i+1}-t_i) + (t_{i+1}-t_i)^2\right\} \\ &= \sum_i \left\{3(t_{i+1}-t_i)^2 - 2(t_{i+1}-t_i)^2 + (t_{i+1}-t_i)^2\right\} \\ &= 2\sum_i (t_{i+1}-t_i)^2 \leq 2\max_i (t_{i+1}-t_i)\sum_i (t_{i+1}-t_i) = 2|\mathcal{P}_n|\, t \to 0\end{aligned} \tag{0.352}$$

One can show that the convergence is even stronger, it is almost sure: $\lim_n Q_n = t$. It is remarkable that, although Q_n is random for any finite n, its limit is not!

This lemma partly justifies the heuristic idea that

$$|dB| \simeq \sqrt{dt} \tag{0.353}$$

which we will use many times in the future.

If we interpret $x(t) = \int_0^t B(s)dB(s)$ as the limit of Riemann sums as in the ordinary definition of integrals, we have to discretize it and then take the limit. The following theorem will show the nature of the "problem".

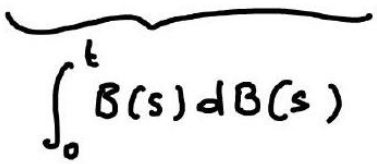
Theorem

Let's take the interval $[0,t](t > 0)$ and partitions $\mathcal{P}_n$ of the interval $\{t_0 = 0 < t_1 < t_2 \cdots < t_n = t\}$ such that $|\mathcal{P}_n| \equiv \max_i |t_i - t_{i-1}| \to 0$ as $n \to \infty$. Also fix $\lambda \in \mathbb{R}, 0 \leq \lambda \leq 1$ and define

$$X_n \equiv \sum_{i=0}^{n-1} B\left(\lambda t_{i+1} + (1-\lambda)t_i\right)\left[B\left(t_{i+1}\right) - B\left(t_i\right)\right] \tag{0.354}$$

then

$$\text{ms-lim}_{\substack{n\to\infty \\ |\mathcal{P}_n|\to 0}} X_n = \frac{[B(t)]^2}{2} + \left(\lambda - \frac{1}{2}\right)t \tag{0.355}$$



COMMENTS:

We recognize X_n as the Riemann sum corresponding to $x(t)$ where we take an arbitrary intermediate point in $[t_i, t_{i+1}]$. In ordinary calculus the integral does not depend on the location of the intermediate point, however in the stochastic integral there is an unavoidable dependence

on which point we choose. This is one of the most important features of the stochastic calculus with Brownian motion. proof: We introduce a more compact notation: $B_i^\lambda \equiv B\left(\lambda t_{i+1} + (1-\lambda)t_i\right), B\left(t_i\right) \equiv B_i$. Then $X_n = \sum_{i=0}^{n-1} B_i^\lambda \left(B_{i+1} - B_i\right)$. We use now the identity (with B.m. everything is easier with squares or squared differences):

$$\begin{aligned} B_i^\lambda \left(B_{i+1} - B_i\right) &= \left(B_i^\lambda - B_i + B_i\right)\left(B_{i+1} - B_i^\lambda + B_i^\lambda - B_i\right) \\ &= \left(B_i^\lambda - B_i\right)\left(B_{i+1} - B_i^\lambda\right) + \left(B_i^\lambda - B_i\right)^2 + B_i\left(B_{i+1} - B_i^\lambda\right) + B_i\left(B_i^\lambda - B_i\right) \\ &= \left(B_i^\lambda - B_i\right)\left(B_{i+1} - B_i^\lambda\right) + \left(B_i^\lambda - B_i\right)^2 + B_i B_{i+1} - B_i^2 \\ &= \underbrace{\left(B_i^\lambda - B_i\right)\left(B_{i+1} - B_i^\lambda\right)}_{\text{(D)}} + \underbrace{\left(B_i^\lambda - B_i\right)^2}_{\text{(C)}} - \underbrace{\frac{1}{2}\left(B_{i+1} - B_i\right)^2}_{\text{(B)}} + \underbrace{\frac{B_{i+1}^2}{2} - \frac{B_i^2}{2}}_{(A)} \end{aligned} \tag{0.356}$$

Let's calculate all the terms: (A) $\sum_{i=0}^{n-1}\left(\frac{B_{i+1}^2}{2} - \frac{B_i^2}{2}\right) = \frac{1}{2}\left(B_n^2 - B_0^2\right) = \frac{B^2(t)}{2}$ (B) $-\frac{1}{2}\sum_{i=0}^{n-1}\left(B_{i+1} - B_i\right)^2 \xrightarrow{\text{ms-limit}} -\frac{t}{2}$ (lemma) (C) $\sum_{i=0}^{n-1}\left(B_i^\lambda - B_i\right)^2 \xrightarrow{\text{ms-limit}} \lambda t$ (use the lemma) (D) We have to show that the term (D) is zero in the ms-limit:

$$\begin{aligned} \mathbb{E}\left[\left(\sum_{i=0}^{n-1}\left(B_i^\lambda - B_i\right)\left(B_{i+1} - B_i^\lambda\right)\right)^2\right] &= \sum_{i=0}^{n-1}\mathbb{E}\left[\left(B_i^\lambda - B_i\right)^2\right]\mathbb{E}\left[\left(B_{i+1} - B_i^\lambda\right)^2\right] \\ &= \sum_{i=0}^{n-1}\lambda\left(t_{i+1} - t_i\right)\cdot(1-\lambda)\left(t_{i+1} - t_i\right) \\ &\leq \lambda(1-\lambda)\max_j\left(t_{j+1} - t_j\right)\sum_{i=0}^{n-1}\left(t_{i+1} - t_i\right) \leq \lambda(1-\lambda)\left|\mathcal{P}_n\right| t \to 0 \text{ as } n \to \infty \end{aligned} \tag{0.357}$$

The theorem shows that

$$\int_0^t B(s)dB(s) = \frac{B^2(t)}{2} + \left(\lambda - \frac{1}{2}\right)t \tag{0.358}$$

so it does depend in general on the intermediate point that we choose. The main choices are: (I) $\int_0^t B(s)dB(s) = \frac{B^2(t)}{2} - \frac{t}{2}$ Itô integral, $\lambda = 0$ (S) $\int_0^t B(s)dB(s) = \frac{B^2(t)}{2}$ Stratonovich integral, $\lambda = \frac{1}{2}$

IMPORTANT COMMENTS:

(1) Why should we use Itô? Since t represents time and because we do not know what value B will get in the following interval $[t_i, t_{i+1}]$, we prefer to select the known value in the approximation, i.e. $B\left(t_i\right)$. This is the choice in (I).

From eq. (32)

$$\mathbb{E}\left[\int_0^t B(s)dB(s)\right] = 0 \tag{0.359}$$

So (I) has the strange property that that it does not follow ordinary calculus, but it is handy because one can show that $\mathbb{E}[B(t)dB(t)] =$

$\mathbb{E}[B(t)]\mathbb{E}[dB(t)] = 0$. In general for Itô integrals:

$$E\left[\int \sigma dB\right] = \int E[\sigma]E[dB] = 0 \tag{0.360}$$

In the following we will always use the Itô prescription when considering SDEs of the form (28).

Notice that if the SDE is with additive noise (eq. (27)) there is no need to introduce any intermediate prescription. If we use a function $\sigma(x)$, instead of $B(s)$, and we define $\int_0^t \sigma(x)dB(s)$ as in eq. (28b), in general $\sigma(x)$ will depend on the B.m. $B(s)$ for $s \leq t$ and we do not know at time t its future value at times $\tau > t$. We don't want σ to depend on $B(\tau) - B(s), \forall \tau > s$. All these functions $\sigma(x)$, which depend only on the information available up to time t (so they are indep. of $B(\tau) - B(s), \forall \tau > s$), are called non-anticipating functions. We will always use these functions. If σ is non-anticipating, the Itô stochastic integral ($\lambda = 0$) of the function $\sigma(x)$ is defined as

$$\int_0^t \sigma(s)dB(s) = \lim_{n\to\infty}\left(\sum_{i=0}^{n-1} \sigma\left(t_i\right)\left[B\left(t_{i+1}\right) - B\left(t_i\right)\right]\right) \tag{0.361}$$

One can also show that (σ non-anticipating)

$$\left\langle\left(\int_0^t \sigma(s)dB(s)\right)^2\right\rangle = \int_0^t ds\left\langle\sigma(s)^2\right\rangle \tag{0.362}$$

(See Gardiner p. 84): ms-lim $\sum_{i=0}^{n-1} \sigma_i^2 \left(B_{i+1} - B_i\right)^2 = \int_0^t ds\sigma(s)^2$ (2) The advantage with the Stratonovich choice ($\lambda = \frac{1}{2}$) is that one can use ordinary calculus, but in this case

$$\mathbb{E}\left[\int_0^t B(s)dB(s)\right] = \frac{t}{2} \tag{0.363}$$

So the B.m. is correlated to the following times.

The dependence on the intermediate point is clear even when calculating the expected value $\mathbb{E}\left[\int_0^t B(s)dB(s)\right]$. The discretization gives ($t_0 = 0, t_n = t$)

$$\begin{aligned}
&\mathbb{E}\left[\sum_{i=0}^{n-1} B\left(t_i + \lambda\left(t_{i+1} - t_i\right)\right)\left(B\left(t_{i+1}\right) - B\left(t_i\right)\right)\right] = \\
&= \sum_i \mathbb{E}\left[B\left(t_i + \lambda\left(t_{i+1} - t_i\right)\right)B\left(t_{i+1}\right)\right] - \sum_i \mathbb{E}\left[B\left(t_i + \lambda\left(t_{i+1} - t_i\right)\right)B\left(t_i\right)\right] \\
&= \sum_{i=0}^{n-1}\left(t_i + \lambda\left(t_{i+1} - t_i\right) - t_i\right) = \lambda t
\end{aligned} \tag{0.364}$$

Exercise: Assume that the stochastic process $g(t)$ depends on the B.m. $B(s)$ for any $s < t$, so g is non-anticipating. Show that $\mathbb{E}\left[\left(\int_0^t g(s)dB(s)\right)^2\right] = \mathbb{E}\left[\int_0^t g^2(s)ds\right]$ if we use the Itô convention. Hint: use the discretization $\sum_{i=0}^{n-1} g\left(t_i\right)\left(B\left(t_{i+1}\right) - B\left(t_i\right)\right)$ and, after all the calculations, take the limit $n \to \infty$.

Itô Calculus

We have seen that the Brownian motion may lead to a change in the usual calculus. In the following we only show what are the new differentiation rules when using the Itô prescription and the finding that $\Delta B \simeq \sqrt{\Delta t}$ Let's assume that $u(B(t), t)$, then

$$\begin{aligned}\Delta u = u(B(t+\Delta t), t+\Delta t) - u(B(t), t) &\overset{\downarrow}{=} \frac{\partial u}{\partial t}\Delta t + \frac{\partial u}{\partial B}\Delta B + \frac{1}{2}\frac{\partial^2 u}{\partial B^2}\Delta B^2 + \text{ h.o.t.} \\ &= \left(\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial B^2}\right)\Delta t + \frac{\partial u}{\partial B}\Delta B \quad \leftarrow \text{ " } \Delta B^2 = \Delta t e x t\text{"} \\ &= \left(\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial B^2}\right)\Delta t + \frac{\partial u}{\partial B}\Delta B\end{aligned} \tag{0.365}$$

this term is not present in ordinary calculus and is due to the fact that $|\Delta B| \simeq \sqrt{\Delta t}$

The Itô differential rule is

$$du = \left(\frac{\partial u}{\partial t} + \frac{1}{2}\frac{\partial^2 u}{\partial B^2}\right)dt + \frac{\partial u}{\partial B}dB \tag{0.366}$$

Of course, if u does not depend on t, $du = \frac{1}{2}\frac{\partial^2 u}{\partial B^2}dt + \frac{\partial u}{\partial B}dB$. Example: $u(B) = B^2$, then $dB^2 = dt + 2BdB$. If we then integrate both sides $\int_{t_1}^{t_2} d\left(B^2\right) = B^2(t_2) - B^2(t_1) = t_2 - t_1 + 2\int_{t_1}^{t_2} B(s)dB(s)$ we get

$$\int_{t_1}^{t_2} B(s)dB(s) = \frac{B^2(t_2) - B^2(t_1)}{2} - \frac{t_2 - t_1}{2} \tag{0.367}$$

which is in agreement with eq. (I)

Exercise: 1) Calculate the Itô differential for B_t^n and show that $dB_t^n = nB_t^{n-1}dB_t + \frac{n(n-1)}{2}B_t^{n-2}dt$ and $\int_0^t B^n dB = \frac{B_t^{n+1}}{n+1} - \frac{n}{2}\int_0^t B(s)^{n-1}ds$ 2) By using the Itô differential of $Y(B,t) = e^{\lambda B(t) - \frac{\lambda^2}{2}t}$ and that $B(0) = 0$, show that $Y(t) = Y(B,t)$ solves the Itô SDE

$$\begin{cases} dY(t) &= \lambda Y(t)dB(t) \\ Y(0) &= 1 \end{cases} \tag{0.368}$$

Show that $\langle Y(t)\rangle = 1 \quad \forall t \geqslant 0$ and $P(y,t) = \frac{e^{-\frac{\left(\ln y + \frac{\lambda^2 t}{2}\right)^2}{2\lambda^2 t}}}{\sqrt{2\pi\lambda^2 t}}y$. This is called log-normal distribution.

Itô's chain rule (Itô's formula)

Suppose that $X(t)$ is a stoch. process which satisfies the SDE

$$dx(t) = \mu(x,t)dt + \sigma(x,t)dB(t) \tag{0.369}$$

where the SDE is interpreted with the Itô prescription; then if $u(x,t) \in C_t^1, \in C_x^2$ then the stochastic process u satisfies the SDE:

$$du = \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\mu + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\sigma^2\right)dt + \frac{\partial u}{\partial x}\sigma dB \tag{0.370}$$

Indeed, we use the simple rules: $dtdB = O\left(dt^{3/2}\right), dB^2 = dt$

$$du = \frac{\partial u}{\partial t}dt + \frac{\partial u}{\partial x}dx + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}dx^2 + \text{ h.o.t.} \tag{0.371}$$

$$\text{however } dx^2 = (\mu dt + \sigma dB)^2 = \mu^2 dt^2 + 2\mu\sigma dt dB + \sigma^2 dB^2 = \sigma^2 dt \tag{0.372}$$

then

$$\begin{aligned} du &= \frac{\partial u}{\partial t}dt + \frac{\partial u}{\partial x}(\mu dt + \sigma dB) + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\sigma^2 dt \\ &= \left(\frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\mu + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\sigma^2\right)dt + \frac{\partial u}{\partial x}\sigma dB \text{ as in (35)} \end{aligned} \tag{0.373}$$

Exercise: 1) The stoch. proc. $x(t)$ satisfies the Itô SDE (This process is called geometric Brownian motion).

$$\begin{cases} dx = \dfrac{x}{2}dt + xdB \\ x(0) = 1 \end{cases} \tag{0.374}$$

Show that the process $y = \ln x$ satisfies the Itô SDE

$$\begin{cases} dy = dB \\ y(0) = 0 \end{cases} \tag{0.375}$$

and therefore the solution of the original SDE is $x(t) = e^{B(t)}$. 2) Itô formula for 2 variables:

Assume that the two processes $x(t)$ and $y(t)$ satisfy the two Itô SDEs $dx = \mu_x dt + \sigma_x dB$ and $dy = \mu_y dt + \sigma_y dB$. By using the Itô rules, show that if $u(x,y) \in C^2(x,y)$ then $du = \left(\frac{\partial u}{\partial x}\mu_x + \frac{\partial u}{\partial y}\mu_y + \frac{1}{2}\frac{\partial^2 u}{\partial x^2}\sigma_x^2 + \frac{1}{2}\frac{\partial^2 u}{\partial y^2}\sigma_y^2 + \frac{\partial^2 u}{\partial x \partial y}\sigma_x\sigma_y\right)dt + \left(\frac{\partial u}{\partial x}\sigma_x + \frac{\partial u}{\partial y}\sigma_y\right)dB$ Take $u(x,y) = xy$, then one can write

$$d(xy) = \left(x\mu_y + y\mu_x + \sigma_x\sigma_y\right)dt + \left(x\sigma_y + y\sigma_x\right)dB \tag{0.376}$$

and deduce the correlation between the two processes x and y 3) The Ornstein-Uhlenbeck process is defined by the SDE:

$$\begin{cases} dx = -\mu x dt + \sigma dB \\ x(0) = x_0 \end{cases} \tag{0.377}$$

In order to solve the SDE, show that the SDE of $y(t) = e^{\mu t}x(t)$ is $dy = \sigma e^{\mu t}dB$, hence $y(t) = y(0) + \sigma\int_0^t e^{\mu s}dB(s)$ and finally

$$x(t) = e^{-\mu t}\left(x_0 + \sigma\int_0^t e^{\mu s}dB(s)\right) \tag{0.378}$$

Ex: Find the solution of the SDE $dx = (\eta - \mu x)dt + \sigma dB$. Of course,

$\mathbb{E}(x(t)) = x_0 e^{-\mu t}$. We calculate now $\left\langle x^2(t) \right\rangle$.

$$\begin{aligned} d\left(x^2\right) &= 2xdx + dx^2 = 2x(-\mu x dt + \sigma dB) + (-\mu x dt + \sigma dB)^2 \\ &= \left(-2\mu x^2 + \sigma^2\right) dt + 2\sigma x dB \\ \frac{d}{dt}\left\langle x^2 \right\rangle &= -2\mu \left\langle x^2 \right\rangle + \sigma^2 + 2\sigma \left\langle x \frac{dB}{dt} \right\rangle = -2\mu \left\langle x^2 \right\rangle + \sigma^2 \\ \left\langle x(t)^2 \right\rangle &= \frac{\sigma^2}{2\mu} + \left(x_0^2 - \frac{\sigma^2}{2\mu}\right) e^{-2\mu t} \end{aligned} \tag{0.379}$$

Thus $\mathrm{Var}[x(t)] = \left\langle x(t)^2 \right\rangle - \langle x(t) \rangle^2 = \frac{\sigma^2}{2\mu}\left(1 - e^{-2\mu t}\right)$

For a stoch. proc. like $x(t)$ we can calculate the auto-correlation $c(t,s) = \langle x(t)x(s) \rangle - \langle x(t) \rangle \langle x(s) \rangle$. As you see from eq. (36), we have to calculate averages of this kind

$$\mathbb{E}\left[\int_0^t G\left(t'\right) dB\left(t'\right) \int_0^s H\left(s'\right) dB\left(s'\right)\right] \tag{0.380}$$

Where G and H are both cont. and non-anticipating. As usual we have to discretize: take $t > s, (n > m)$

$$\begin{aligned} &\mathbb{E}\left[\sum_{i=0}^{n-1} G_i \left(B_{i+1} - B_i\right) \sum_{j=0}^{m-1} H_j \left(B_{j+1} - B_j\right)\right] = \\ =&\mathbb{E}\left[\sum_{i=0}^{m-1} G_i \left(B_{i+1} - B_i\right) \sum_{j=0}^{m-1} H_j \left(B_{j+1} - B_j\right)\right] + \mathbb{E}\left[\sum_{i=m}^{n-1} \ldots \sum_{j=0}^{m-1} \ldots\right] \\ =&\mathbb{E}\left[\sum_{i=0}^{m-1} G_i H_i \left(B_{i+1} - B_i\right)^2\right] + 2\mathbb{E}\left[\sum_{i \neq j}^{m-1} G_i \left[B_{i+1} - B_i\right] H_j \left[B_{j+1} - B_j\right]\right] = \\ =&\mathbb{E}\left[\sum_{i=0}^{m-1} G_i H_i \left(B_{i+1} - B_i\right)^2\right] \end{aligned} \tag{0.381}$$

now by taking the limit $m \to \infty$

$$\longrightarrow \mathbb{E}\left[\int_0^s G\left(s'\right) H\left(s'\right) ds'\right] = \int_0^s \mathbb{E}\left[G\left(s'\right) H\left(s'\right)\right] ds' \tag{0.382}$$

If we re-do the calculations for $t < s$, we can convince ourselves that

$$\mathbb{E}\left[\int_0^t G\left(t'\right) dB\left(t'\right) \int_0^s H\left(s'\right) dB\left(s'\right)\right] = \int_0^{t \wedge s} \mathbb{E}\left[G\left(s'\right) H\left(s'\right)\right] ds' \tag{0.383}$$

Now let's use eq. (39) to calculate the auto-correlation function of the O-U process, whose solution is in eq. (36)

$$\begin{aligned} \mathbb{E}[x(t)x(s)] &= \mathbb{E}\left[e^{-\mu t}\left(x_0 + \sigma \int_0^t e^{\mu t'} dB\left(t'\right)\right) e^{-\mu s}\left(x_0 + \sigma \int_0^s e^{\mu s'} dB\left(s'\right)\right)\right] \\ &= x_0^2 e^{-\mu(t+s)} + \sigma^2 e^{-\mu(t+s)} \int_0^{t \wedge s} e^{2\mu s'} ds' \\ &= x_0^2 e^{-\mu(t+s)} + \frac{\sigma^2}{2\mu} e^{-\mu(t+s)}\left(e^{2\mu(t \wedge s)} - 1\right) \\ &= x_0^2 e^{-\mu(t+s)} + \frac{\sigma^2}{2\mu}\left(e^{-\mu|t-s|} - e^{-\mu(t+s)}\right) \end{aligned} \tag{0.384}$$

And therefore the (connected) auto-correlation function is

$$c(t,s) = \frac{\sigma^2}{2\mu}\left(e^{-\mu|t-s|} - e^{-\mu(t+s)}\right) \tag{0.385}$$

If we start from some distribution $p(x_0)$ for the initial conditions, we get

$$c(t,s) = \mathrm{Var}(x_0)\, e^{-\mu(t+s)} + \frac{\sigma^2}{2\mu}\left(e^{-\mu|t-s|} - e^{-\mu(t+s)}\right) \tag{0.386}$$

Notice that, if we let $t, s \to \infty$ but $t - s$ is fixed, then from (40) we get

$$C_{\text{stat}}(|t-s|) = \frac{\sigma^2}{2\mu} e^{-\mu|t-s|} \tag{0.387}$$

which only depends on $|t - s|$. This is the stationary autocorrelation function of the O.-U. process which does not depend on any initial condition!

Gaussian Integrals continued **First Semester**

Lecture 11

Date: 2025-10-03 Profesor: Azaele Sandro

0.11 Gaussian Integrals continued

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}+bx}dx = \sqrt{\frac{2\pi}{a}}e^{\frac{b^2}{2a}} \quad a>0, b\in\mathbb{C} \tag{0.388}$$

$$\varphi(k) = \int e^{ikx}p(x)dx = \left\langle e^{ikx}\right\rangle \tag{0.389}$$

$$(-i)^n \frac{d^n\varphi}{dk^n}\bigg|_{k=0} = \langle x^n\rangle \tag{0.390}$$

$$\int_{-\infty}^{+\infty} \frac{1}{\sqrt{2\pi\sigma^2}}e^{-\frac{x^2}{2\sigma^2}}e^{ikx}dx = e^{-\frac{\sigma^2k^2}{2}} \tag{0.391}$$

Because of eq. (5)

$$\langle x\rangle = -\,i\frac{d}{dk}e^{-\frac{\sigma^2k^2}{2}}\bigg|_{k=0} = 0 \tag{0.392}$$

Important Gaussian integrals: $\langle x^n\rangle = (-i)^n \frac{d^n}{dk^n}e^{-\frac{\sigma^2k^2}{2}}\Big|_{k=0} = 0$ if n is odd (by symmetry). However

$$\left\langle x^4\right\rangle = \frac{d^4}{dk^4}e^{-\frac{\sigma^2k^2}{2}}\bigg|_{k=0} = \left[\sigma^4\left(3-6k^2\sigma^2+k^4\sigma^4\right)e^{-\frac{\sigma^2k^2}{2}}\right]_{k=0} = 3\sigma^4 = \frac{1}{\sqrt{2\pi\sigma^2}}\int_{-\infty}^{+\infty} e^{-\frac{x^2}{2\sigma^2}}x^4dx. \tag{0.393}$$

If we want to calculate $\langle x^n\rangle$, we better start from

$$\int_{-\infty}^{+\infty} e^{-\frac{ax^2}{2}}dx = \sqrt{\frac{2\pi}{a}} \tag{0.394}$$

We differentiate both sides wrt a: once

$$\int_{-\infty}^{+\infty} x^2e^{-\frac{ax^2}{2}}dx = \frac{\sqrt{2\pi}}{a^{3/2}} \to \left\langle x^2\right\rangle \tag{0.395}$$

twice

$$\int_{-\infty}^{+\infty} x^4e^{-\frac{ax^2}{2}}dx = \frac{3\sqrt{2\pi}}{a^{5/2}} \tag{0.396}$$

$n/2$ times, n is even

$$\int_{-\infty}^{+\infty} x^ne^{-\frac{ax^2}{2}}dx = \frac{(n-1)!!\sqrt{2\pi}}{a^{(n+1)/2}} \tag{0.397}$$

From this find the expression of $\langle x^n\rangle$ as a function of σ and n (even).

Multidimensional Gaussian Integrals

Example:

$$\int_{-\infty}^{+\infty} dx_1\int_{-\infty}^{+\infty} dx_2e^{-\frac{3}{2}\left(x_1^2+x_2^2\right)+x_1x_2} = ? \tag{0.398}$$

Ex: write down the exponent in the form $-\frac{1}{2}\vec{x}^\top A\vec{x}$. More generally,

$$Z(A) = \int_{\mathbb{R}^m} d^m x e^{-\frac{1}{2}\vec{x}^\top A\vec{x}} \tag{0.399}$$

Where $\vec{x} = (x_1, \ldots, x_m)$ and the matrix A is diagonalizable with strictly positive eigenvalues (positive definite). Then there exist an orthogonal matrix $O \quad (\Rightarrow OO^\top = O^\top O = \mathbb{1})$ such that we can define $\vec{y} = O\vec{x}$ and $OAO^\top = \Lambda$

$$\Lambda = \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_m \end{pmatrix} \quad \lambda_i > 0 \quad i = 1, 2, \ldots m \tag{0.400}$$

It follows that

$$\vec{x}^\top A\vec{x} = \vec{x}^\top O^\top \Lambda O\vec{x} = \vec{y}^\top \Lambda\vec{y} \tag{0.401}$$

$Z(A) = \int d^m x e^{-\frac{1}{2}\vec{x}^\top A\vec{x}} = \int d^m y \left|\frac{\partial\vec{x}}{\partial\vec{y}}\right| e^{-\frac{1}{2}\vec{y}^\top\Lambda\vec{y}}$ determinant of the Jacobian: $\left|\frac{\partial\vec{x}}{\partial\vec{y}}\right| = \det(O^\top) = 1$ (show as an exercise.)

$$\vec{y}^\top\Lambda\vec{y} = \sum_{ij} y_i\Lambda_{ij}y_j = \sum_{ij} y_i\lambda_i\delta_{ij}y_j = \sum_i \lambda_i y_i^2 \tag{0.402}$$

From this we get

$$= \int_{\mathbb{R}^m} d^m y e^{-\frac{1}{2}\sum_i \lambda_i y_i^2} = \prod_{i=1}^m \int_{-\infty}^{+\infty} dy_i e^{-\frac{1}{2}\lambda_i y_i^2} = \prod_{i=1}^m \sqrt{\frac{2\pi}{\lambda_i}} = \frac{(2\pi)^{m/2}}{\sqrt{\lambda_1 \cdots \lambda_m}} \tag{0.403}$$

$\det(A) = \det\left(O^\top\Lambda O\right) = \det(\Lambda)(\det O)^2 = \det\Lambda = \lambda_1 \cdots \lambda_m$

Hence

$$Z(A) = \frac{(2\pi)^{m/2}}{\sqrt{\det A}} = \int_{\mathbb{R}^m} d^m x e^{-\frac{1}{2}\vec{x}^\top A\vec{x}} \tag{0.404}$$

By using (8) show that

$$\int_{-\infty}^{+\infty} dx_1 \int_{-\infty}^{+\infty} dx_2 e^{-\frac{3}{2}\left(x_1^2+x_2^2\right)+x_1x_2} = \frac{\pi}{\sqrt{2}} \tag{0.405}$$

Exercise: Let $p(x, y) = \frac{\sqrt{\det A}}{2\pi} e^{-\frac{1}{2}\left(a_{11}x^2+2a_{12}xy+a_{22}y^2\right)}$ where $a_{11}, a_{22} > 0$. Show that $q(x) = \int p(x, y)dy$ is still a Gaussian distribution. Find the corresponding variance of x. This is also true for m-dimension Gaussian variables.

We want now to calculate

$$Z(A, \vec{b}) = \int d^m x e^{-\frac{1}{2}\vec{x}^\top A\vec{x}+\vec{x}^\top\cdot\vec{b}} \tag{0.406}$$

we use the same strategy we used before:

$$\vec{\nabla}_x\left(-\frac{1}{2}\vec{x}^\top A\vec{x} + \vec{x}^\top\cdot\vec{b}\right) = -A\vec{x} + \vec{b} = 0 \Rightarrow \vec{x} = A^{-1}\vec{b} \quad (\text{if } \det A \neq 0) \tag{0.407}$$

We introduce

$$\begin{aligned} \vec{y} &= \vec{x} - A^{-1}\vec{b} \\ -\frac{1}{2}\vec{x}^\top A\vec{x} + \vec{x}^\top \cdot \vec{b} &= -\frac{1}{2}\vec{y}^\top A\vec{y} + \frac{\vec{b}^\top A^{-1}\vec{b}}{2} \quad \text{(do the calculation).} \end{aligned} \tag{0.408}$$

Hence

$$Z(A,\vec{b}) = \int_{\mathbb{R}^m} d^m y e^{-\frac{1}{2}\vec{y}^\top A\vec{y} + \frac{\vec{b}^\top A^{-1}\vec{b}}{2}} = e^{\frac{\vec{b}^\top A^{-1}\vec{b}}{2}} Z(A,0) \tag{0.409}$$

$$Z(A,\vec{b}) = \frac{(2\pi)^{m/2}}{\sqrt{\det A}} e^{\frac{\vec{b}^\top A^{-1}\vec{b}}{2}} \tag{0.410}$$

Eq. (10) allows to find the charact. function of the multivariate Gaussian distrib.

$$p(\vec{x}) = \frac{1}{Z(A,0)} e^{-\frac{1}{2}\vec{x}^\top A\vec{x}} \tag{0.411}$$

$$\int_{\mathbb{R}^m} d^m x p(x) e^{i\vec{k}\cdot\vec{x}} = e^{-\frac{\vec{k}^\top A^{-1}\vec{k}}{2}} = \varphi(k) \tag{0.412}$$

What is the meaning of A^{-1}? The definition of the ch. f. in the multidim. case is:

$$\varphi(\vec{k}) = \int d^m x e^{i\vec{k}\cdot\vec{x}} p(\vec{x}) \quad \vec{k} = (k_1, k_2, \ldots, k_m) \tag{0.413}$$

therefore we derive

$$(-i)^s \frac{\partial^s}{\partial k_i \partial k_j \cdots \partial k_l} \varphi(\vec{k})\Big|_{\vec{k}=0} = \int d^m x x_i x_j \cdots x_l p(\vec{x}) = \langle x_i x_j \cdots x_l \rangle \tag{0.414}$$

Let's calculate the 2-point correlation function for a Gaussian distr.

$$\langle x_i x_j \rangle = (-i)^2 \frac{\partial}{\partial k_i} \frac{\partial}{\partial k_j} e^{-\frac{\vec{k}^\top A^{-1}\vec{k}}{2}}\Big|_{\vec{k}=0} = \left(A^{-1}\right)_{ij} \tag{0.415}$$

A^{-1} is the 2-point correlation function between a pair of Gauss. r.v. When A^{-1} is a diagonal matrix, we say that the vars are uncorrelated.

In the previous example:

$$A = \begin{pmatrix} 3 & -1 \\ -1 & 3 \end{pmatrix} \quad A^{-1} = \frac{1}{8}\begin{pmatrix} 3 & 1 \\ 1 & 3 \end{pmatrix} \tag{0.416}$$

hence

$$\langle x_1^2 \rangle = \frac{3}{8} = \langle x_2^2 \rangle \quad \langle x_1 x_2 \rangle = \frac{1}{8} = \langle x_2 x_1 \rangle \tag{0.417}$$

Notice that, because of symmetry, the s-point correl. funct. for s-variable (s is odd) is zero (the Gaussian remains unchanged when $\vec{x} \to -\vec{x}$).

What happens when we calculate $\langle x_i x_j \ldots x_l \rangle$? Should we do all the derivatives like in eq. (12)? No! If the vars are Gaussian then we can use:

Wick's Theorem

Any correlation between an even number of zero-mean Gaussian r.v. can be written down as a sum of products of 2-point correlation functions $\left(A^{-1}\right)$. For instance:

$$\langle x_a x_b x_c x_d \rangle = \langle x_a x_b \rangle \langle x_c x_d \rangle + \langle x_a x_c \rangle \langle x_b x_d \rangle + \langle x_a x_d \rangle \langle x_b x_c \rangle \tag{0.418}$$

In general

$$\underbrace{\langle x_i x_j \cdots x_m x_n \rangle}_{s \text{ vars}} = \sum_p \left(A^{-1}\right)_{i_p j_p} \cdots \left(A^{-1}\right)_{m_p n_p} \tag{0.419}$$

where the sum is over all possible pairings of s indexes, i.e. over all ways of grouping s (even) indexes $i, j \ldots, m, n$ into pairs (counting pairs even when indexes are equal). Exercise: show that

$$\begin{aligned} \left\langle x_1^2 x_2^2 \right\rangle &= \langle x_1 x_1 \rangle \langle x_2 x_2 \rangle + 2 \langle x_1 x_2 \rangle^2 = \frac{3}{8} \cdot \frac{3}{8} + 2 \left(\frac{1}{8}\right)^2 = \frac{11}{64} \\ \left\langle x_1^4 \right\rangle &= 3 \left\langle x_1^2 \right\rangle^2 = 3 \left(\frac{3}{8}\right)^2 = \frac{27}{64} \end{aligned} \tag{0.420}$$

J. Zinn-Justin, Quantum Field Theory and Critical Phenomena (ch. 1).

Important results obtained with characteristic functions

If we are given the joint probability density function $p(x_1, x_2)$ and it happens that $p(x_1, x_2) = p_1(x_1)p_2(x_2)$ then the two vars are independent. If, on top of this, $p_1 = p_2$, then we say that the two r.v. are independent and identically distributed (i.i.d.).

If we are given two r.v. that are i.i.d. can we calculate the distribution of their sum? If $x_1 \sim q(x)$ and $x_2 \sim q(x)$ what is the distribution of $x = x_1 + x_2$?

Laplace method **First Semester**

Lecture 12

Date: 2025-10-14 Profesor: Azaele Sandro

0.12 Laplace method

$$I(\lambda) \simeq g(x_0)\, e^{\lambda f(x_0)} \sqrt{\frac{2\pi}{\lambda \left| f''(x_0) \right|}} \tag{0.421}$$

interior max $I(\lambda) \sim \lambda^{-1/2} e^{\lambda f(x_0)}$ endpoint (not flat) $\quad I(\lambda) \sim \lambda^{-1} e^{\lambda f(x_0)}$

Lp-norm in real analysis

The quantity

$$\|g\|_p := \left(\int_a^b |g(t)|^p dt \right)^{1/p} \qquad p > 0 \tag{0.422}$$

is called p-norm when the integral exists (in Lebesgue sense). We want to study the behavior of $\|g\|_p$ as $p \to \infty$. We assume that g has a unique maximum in t_0 which is an interior point, and $g \in C^4(a,b)$. We first study

$$I(p) \equiv \int_a^b |g(t)|^p dt \quad \|g\|_p = I(p)^{1/p} \tag{0.423}$$

and

$$I(p) = \int_a^b e^{p \ln |g(t)|} dt \tag{0.424}$$

When we applied the Laplace method we have always assumed that f is continuously differentiable. However, if g vanishes somewhere in $[a,b]$ then $\ln|g| \to -\infty$. However, every neighborhood of points where $g = 0$ will yield a negligible contribution to the integral (i.e. to I for $p \gg 1$).

Thus such discontinuities can be neglected. Now we use eq. (22) from the previous lecture:

$$\begin{aligned} I(p) &= e^{p \ln |g(t_0)|} \sqrt{\frac{2\pi \left| g(t_0) \right|}{p \left| g''(t_0) \right|}} \left(1 + O\left(\frac{1}{p} \right) \right) \\ &= \left| g(t_0) \right|^p \sqrt{\frac{2\pi \left| g(t_0) \right|}{p \left| g''(t_0) \right|}} \left(1 + O\left(\frac{1}{p} \right) \right) \text{ as } p \to \infty \end{aligned} \tag{0.425}$$

Obs: $\quad a > 0 \quad a^{1/p} p^{-\frac{1}{2p}} = e^{\frac{\ln a}{p}} e^{-\frac{\ln p}{2p}}$

$$I(p)^{1/p} = \left| g(t_0) \right| \left(\frac{2\pi |g|}{p \left| g'' \right|} \right)^{\frac{1}{2p}} + \ldots = \left| g(t_0) \right| \left(1 - \frac{\ln p}{2p} + O\left(\frac{1}{p} \right) \right) \tag{0.426}$$

hence

$$\|g\|_p = \max_{t \in [a,b]} |g(t)| \left\{ 1 - \frac{\ln p}{2p} + \cdots \right\} \text{ as } p \to \infty \tag{0.427}$$

which justifies the usual definition

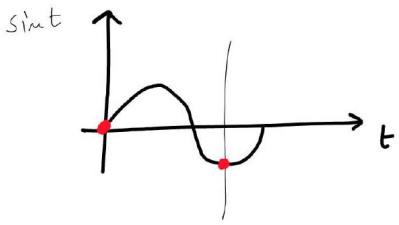
$$\|g\|_\infty = \max_{t\in[a,b]} |g(t)| \tag{0.428}$$

Example

Consider the integral

$$\int_0^{\frac{3\pi}{2}} e^{-\lambda \sin t} f(t)dt \quad \text{as} \quad \lambda \to \infty \tag{0.429}$$

where f is cont. and diff. in $\left[0, \frac{3\pi}{2}\right]$.



We want to consider the contributions from the endpoint minima $t = 0, t = \frac{3\pi}{2}$. For this we write

$$I(\lambda) = \underbrace{\int_0^{\pi/2} e^{-\lambda \sin t} f(t)dt}_{I_1} + \underbrace{\int_{\pi/2}^{3\pi/2} e^{-\lambda \sin t} f(t)dt}_{I_2} \tag{0.430}$$

eqeq(24) left end point

$$I_1 \simeq f(0)\frac{e^{-\lambda \sin(0)}}{\lambda \cos(0)} = \frac{f(0)}{\lambda} \text{ as } \lambda \to \infty \tag{0.431}$$

eqeq(23) flat endpoint

$$I_2 \simeq f\left(\frac{3\pi}{2}\right) e^{\lambda} \sqrt{\frac{\pi}{2\lambda \left|\sin\left(\frac{3\pi}{2}\right)\right|}} = f\left(\frac{3\pi}{2}\right) e^{\lambda} \sqrt{\frac{\pi}{2\lambda}} \tag{0.432}$$

Hence the leading contribution comes from I_2 and

$$I(\lambda) \simeq f\left(\frac{3\pi}{2}\right) e^{\lambda} \sqrt{\frac{\pi}{2\lambda}} \quad \text{as} \quad \lambda \to \infty \tag{0.433}$$

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

Ex: Calculate the leading contribution to

$$\int_0^{\pi} e^{-\lambda \sin t} f(t)dt \quad \text{as } \lambda \to \infty \tag{0.434}$$

0.13 Review of Dynamical Systems

In many applications (physics, biology, chemistry...) one has to study nonlinear systems of (autonomous) ODEs:

$$\begin{cases} \dot{\vec{x}}(t) = \vec{f}(\vec{x}(t)) \\ \vec{x}(0) = \vec{x}_0 \end{cases} \tag{0.435}$$

where $\vec{x}(t) = (x_1(t), \ldots, x_N(t)) \in U \subseteq \mathbb{R}^N$, U is some open connected set of reals. With any $\vec{x}$ we associate a vector $\vec{f}$, the set of these vectors is called vector field. The domain U, where $\vec{f}$ is supposed to be continuous and differentiable, is called the phase space. The solutions $\vec{x}\,(t, x_0)$ of the system (1) describe smooth curves as t changes: they are called trajectories which are parametric curves in the phase space.

Example:

Let's consider ($N = 1$)

$$\dot{x}(t) = \sin[x(t)] \tag{0.436}$$

In this case the vector field is 1-dim. and coincides with the x-axis.

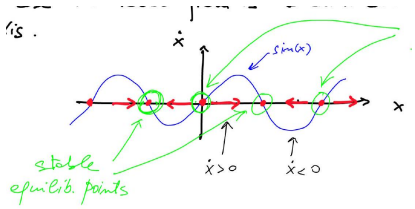


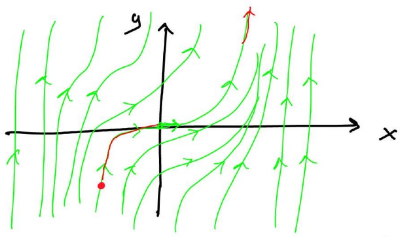
Figure 3: equil. points

In the $N = 2$ case

$$\begin{cases} \dot{x} = 1 \\ \dot{y} = x^2 + y^2 \end{cases} \tag{0.437}$$

the vector field is 2 dim. and we have a map

$$\vec{x} = (x, y) \longrightarrow \vec{f}(\vec{x}) = \left(1, x^2 + y^2\right) \tag{0.438}$$

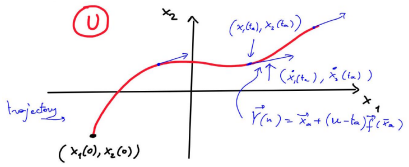


In general the vector field $\vec{f}$ is tangent to a trajectory in every point. In fact, let $\vec{x}(t)$ be a trajectory, then the eq. of a tangent line to the trajectory

at a point $\vec{x}_a \equiv \vec{x}(t_a)$ is

$$\vec{Y}(u) = \vec{x}_a + (u - t_a)\,\dot{\vec{x}}(t_a) = \vec{x}_a + (u - t_a)\,\vec{f}(\vec{x}_a) \tag{0.439}$$

thus $\vec{f}$ is the directional vector of the straight line $\vec{Y}(u)$.



$$N = 2 \begin{cases} \dot{x}_1 = f_1 \\ \dot{x}_2 = f_2 \end{cases} \tag{0.440}$$

By flowing along the vector field, a point traces out the trajectory $\vec{x}(t)$, a curve in the phase space U or a sol. of (2).

A phase portrait is a set of trajectories with the indication of the directions of the vector field. As we cannot solve the system (1) in general, we would like to know at least some properties. Sometimes it is useful to study nullclines, defined as subspaces (or manifolds) where $\dot{x}_i = 0$ for a given i. In $N = 2$ we may get simple curves

$$\dot{x}_1 = 0 \Rightarrow f_1(x_1, x_2) = 0 \text{ possibly } x_2 = g(x_1) \tag{0.441}$$

Two interesting examples

1. Find a solution of $\dot{y} = y^2$ with i.c. $y(0) = 1$.

Can we then find $y(2)$? From $\int \frac{dy}{y^2} = t - c$, $y = \frac{1}{c-t}$, $y(0) = 1 \Rightarrow c = 1$

$$y(t) = \frac{1}{1-t} \quad \to y(2) = -1 \tag{0.442}$$

As $\dot{y}(t) \geqslant 0$, y is an increasing function of time but $y(2) = -1$! Actually, the solution exists only in the interval $(0, 1)$ as it blows up at $t = 1$. Solutions may exist only within finite intervals of time or they may not exist for some initial conditions or may not exist at all.

2. Find a solution of $\dot{y} = \sqrt{y}$ for which $y(0) = 0$. Find $y(2)$.

$$\int \frac{dy}{\sqrt{y}} = 2\sqrt{y} = t - c, \quad y = \frac{(t-c)^2}{4} \text{ but } y(0) = 0, y(t) = \frac{t^2}{4} \tag{0.443}$$

hence $y(2) = 1$. But!

However $y(t) = 0$ satisfies the eq. and the init. cond. Even worse:

$$y(t) = \begin{cases} 0 & 0 \leq t \leq T \quad T \text{ is arbitrary} \\ \dfrac{(t-T)^2}{4} & t > T \qquad\qquad T > 0. \end{cases} \tag{0.444}$$

is a solution with the same initial condition! So there are infinitely many solutions, so asking for $y(2)$ is meaningless. Sol. to init. val problems may not be unique.

Picard's theorem

If $\vec{f}$ is continuous and $\frac{\partial f_i}{\partial x_j}$ are also continuous for all indexes i, j in U, then for any $\vec{x}_0 \in U$ the initial value problem defined in (1) admits a solution on some interval $t \in [-\delta, \delta], \delta > 0$, and this solution is unique.

Obs: in this case trajectories do not intersect.

Fixed points

The fixed points of eq. (1) are the simplest to study as time is not relevant. Indeed, fixed points are the zeros of $\vec{f}$: namely, $\vec{x}^*$ is a fixed point if

$$\vec{f}\left(\vec{x}^*\right) = \overrightarrow{0} \tag{0.445}$$

Warning: even though an ODE has some fixed points, that does not imply that the dynamics (the init. val. solut.) reach them!

Law of large numbers **First Semester**

Lecture 13

Date: 2025-10-07 Profesor: Azaele Sandro

0.14 Law of large numbers

If we are given 2 r.v. x_1, x_2 and their joint prob. p(x_1, x_2) , $then we say that x_1$ and x_2 are indep if.

$$p(x_1, x_2) = p(x_1)\, q(x_2) \tag{0.446}$$

where $x_1 \sim p(x_1)$ and $x_2 \sim q(x_2)$. In general $p \neq q$. Also, if $p = q$, then we say that x_1 and x_2 are independent and identically distributed.

If we are given x_1, x_2 that are i.i.d. what is the distribution of

$$x = x_1 + x_2 \quad x \sim p(x) \tag{0.447}$$

$$p(x) = \int \delta(x - (x_1 + x_2)) p(x_1, x_2)\, dx_1 dx_2 \equiv \langle \delta(x - x_1 - x_2) \rangle \tag{0.448}$$

we select all possible x_1, x_2 s.t. their sum is x. i.i.d.

$$\begin{aligned} &= \int \delta(x - x_1 - x_2)\, q(x_1)\, q(x_2)\, dx_1 dx_2 \\ &= \int q(x - y) q(y) dy \quad \text{it's a convolution.} \end{aligned} \tag{0.449}$$

We can calculate the c.f. of $p(x)$:

$$\varphi(k) \equiv \left\langle e^{ikx} \right\rangle = \int e^{ikx} p(x) dx = \int dx e^{ikx} \delta(x - x_1 - x_2)\, q(x_1)\, q(x_2)\, dx_1 dx_2 \tag{0.450}$$
$$= \int e^{ik(x_1 + x_2)} q(x_1)\, q(x_2)\, dx_1 dx_2 = \left[\varphi_1(k)\right]^2$$

Exerc.: What is the distribution of the sum if they are indep but not ident. distrib.?

- What is the c.f. of distrib. of the sum of n iid?
- Calculate the distrib of $x = x_1 + x_2$ where x_1, x_2 are iid drawn from a) $U([0, 1])$, b) $N(\mu, \sigma)$, c) $\lambda e^{-\lambda x}$.
- Calculate the distribution of the product $x = x_1 x_2$ where x_1, x_2 are positive iid.

The (weak) law of large numbers

If we are given n iid rand. var. whose pdf is $q(x)$ with a c.f. $\varphi_1(k)$, what happens to $X = \frac{1}{n} \sum_i x_i$ as $n \to \infty$?

We assume that the mean of x_i is ($\mu = \int dx q(x) x < \infty$). (See Grimmett & Stirzaker, p. 193, Prob. and Random Processes). proof: Let $\varphi_n(k)$ be the c.f. of the average of the rand. variables

$$\varphi_n(k) \equiv \left\langle e^{ikX} \right\rangle = \left\langle e^{ik \frac{1}{n} \sum_i x_i} \right\rangle = \int e^{\frac{ik}{n} \sum_i x_i} q(x_1) \cdots q(x_n)\, dx_1 \cdots dx_n \tag{0.451}$$

$$= \left(\int e^{i \frac{k}{n} x_1} q(x_1) dx_1 \right) \cdots \left(\int e^{ik \frac{x_n}{n}} q(x_n)\, dx_n \right) = \left(\varphi_1\left(\frac{k}{n}\right) \right)^n \tag{0.452}$$

$$\varphi_1\left(\frac{k}{n}\right) = \int e^{i \frac{k}{n} x} q(x) dx = 1 + \frac{ik}{n} \langle x \rangle + \mathcal{O}\left(\frac{1}{n^2}\right) \text{ as } n \to \infty \tag{0.453}$$

Taylor convergence in distribution from (17)

$$\left(1 + \frac{ik}{n} \tag{0.454}$$

$$langlex\rangle + \ldots^n \xrightarrow[n\to\infty]{} e^{i\mu k} = \int \underbrace{\delta(x-\mu)}_{p(x)=\delta(x-\mu)} e^{ikx} dx \tag{0.455}$$

The strong law of large numbers

Let $x_1 \ldots x_n$ be a sequence of i.i.d. r.v. each with finite mean
mu. Then the empirical average
$frac1n \sum_i x_i$ approaches
mu as $n \to \infty$ (Grimmett, p. 329).

Here the convergence is almost sure.

$$P(\{ \tag{0.456}$$

$$frac1n \sum_{i=1}^{n} x_i \to \mu \text{ as } n \to \infty = 1 \tag{0.457}$$

This Theorem tells us that for large n the sum
$sum_i x_i$ is well approximated by
mun. Of course there will be fluctuations around
mun. A natural question is : what can we say about
$sum_i x_i - n\mu$? How fast do we approach the limit? What about the fluctuations around n
mu? Whenever x_i have finite variance
$sigma^2$:

1. $sum_i x_i -$
   mun is about as big as
   $sqrtn$
2. The distribution of
   $fracsum_i x_i - munsqrtn$ approaches a Gaussian distribution as $n \to \infty$ IRRESPECTIVE of the distribution of x_i.

The claims in a) and b) are the core meaning of the Central Limit Theorem
Let $x_1 \ldots x_n$ be a sequence of i.i.d. r.v. with finite mean
mu and finite (non-zero) variance
$sigma^2$. Then the PDF of

$$\mathrm{Y}_n = \tag{0.458}$$

$$frac \tag{0.459}$$

$$sum_i x_i - \tag{0.460}$$

$$mun \tag{0.461}$$

$$sqrtn\sigma \xrightarrow[n\to\infty]{\text{conv. in distrib.}} N(0,1) \tag{0.462}$$

Obs:

$$\langle Y_n \rangle = \frac{1}{\sqrt{n}\sigma} \left(\sum_i \langle x_i \rangle - \mu n \right) = 0 \tag{0.463}$$

Ex:

$$\mathrm{Var}\left(Y_n\right) = \cdots = 1 \tag{0.464}$$

- Let x_1, x_2 be two i.i.d. Gaussian r.v. such that

$$\langle x_i \rangle = 0, \left\langle x_i^2 \right\rangle = 1, \langle x_1 x_2 \rangle = 0 \quad i = 1, 2 \tag{0.465}$$

  Calculate $\left\langle y_i \right\rangle, \left\langle y_i^2 \right\rangle, \left\langle y_1 y_2 \right\rangle \quad i = 1, 2$ where

$$\begin{cases} y_1 = \rho + \sqrt{1-\rho^2} x_1 \\ y_2 = \rho + \sqrt{1-\rho^2} \left(\gamma x_1 + \sqrt{1-\gamma^2} x_2 \right) \end{cases} \tag{0.466}$$

  where $|\rho| \leqslant 1, |\gamma| \leqslant 1$.

Obs: the definition of Y_n means that it is centered at 0 with a variance that does not depend on n. proof: Let's assume that each r.v. has a p.d.f. $q(x)$ with c.f.
$varphi_1(k)$,
$varphi_n(k)$ is the c.f. of Y_n:

$$\varphi_n(k) = \left\langle e^{ikY_n} \right\rangle = \int e^{ik \frac{\sum_i x_i - \mu n}{\sqrt{n}\sigma}} q\left(x_1\right) \cdots q\left(x_n\right) dx_1 \cdots dx_n = \tag{0.467}$$

$$= \mathrm{e}^{-\frac{ik\mu\sqrt{n}}{\sigma}} \left(\int e^{\frac{ikx}{\sqrt{n}\sigma}} q(x) dx \right)^n = e^{-\frac{ik\mu\sqrt{n}}{\sigma}} (\tag{0.468}$$

$$varphi_1 \left(\frac{k}{} \right. \tag{0.469}$$

$$sqrtn\sigma^n \tag{0.470}$$

As in the previous theorem we can expand
$varphi_1$ as $n \to \infty$

$$\varphi_1 \left(\frac{k}{\sqrt{n}\sigma} \right) = 1 + \frac{ik}{\sqrt{n}\sigma} \langle x \rangle - \frac{k^2}{2n\sigma^2} \left\langle x^2 \right\rangle + O\left(n^{-3/2}\right) = e^{\frac{ik\mu}{\sqrt{n}\sigma} - \frac{k^2}{2n}} \tag{0.471}$$

from (20)

$$\varphi_n(k) = e^{-\frac{ik\mu}{\sigma}\sqrt{n}} e^{\frac{ik\mu}{\sigma}\sqrt{n} - \frac{k^2}{2}} = e^{-\frac{k^2}{2}} \tag{0.472}$$

As we have shown in eq. (6), this is the c.f. of

$$p(x) = \frac{1}{\sqrt{2\pi}} e^{-\frac{x^2}{2}} \equiv N(0,1) \tag{0.473}$$

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

Fokker-Planck equation **First Semester**

Lecture 2

Date: 2025-10-17 Profesor: Azaele Sandro

0.15 Fokker-Planck equation

Derivation of the Fokker-Planck equation for a general Langevin equation (Itô prescription)

We start from a stochastic process defined via the Langevin equation (Itô)

$$dx(t) = \mu(x(t), t)dt + \sigma(x(t), t)dB(t) \tag{0.474}$$

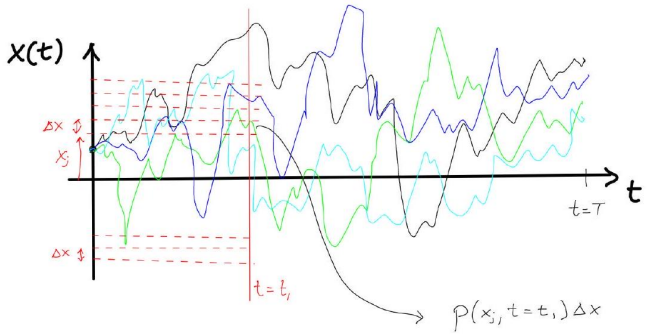
where $x(0) = x_0$ (or a generic initial PDF). $B(t)$ is a standard Brownian process. An alternative way to write eq. (1) is the "pseudo-equation"

$$\dot{x} = \mu(x, t) + \sigma(x, t)\xi(t) \tag{0.475}$$

Where $\langle \xi(t) \rangle = 0$ and $\langle \xi(t')\, \xi(t) \rangle = \delta(t' - t)$. We used the suggestive relation " $\frac{dB}{dt} = \xi$ ", even though this is only a formal, notational expression.

Eq. (1) defines the process $x(t)$ so we can use the eq. to generate as many trajectories as we wish. Let us assume that we have generated a large number N of paths from time $t = 0$ to $t = T > 0$. How can we calculate the probability that $x(t)$ gets a value between x and $x + \Delta x$ (a PDF) at time t?

From the computational point of view this is relatively easy: We have



to count how many paths fall in the interval $[x, x + \Delta x)$ at time $t = t_1$ as x varies in the domain of definition of the process $x(t)$. If we use the indicator function, I, defined as

$$I(a, A) = \begin{cases} 1 a \in A \\ 0 a \notin A \end{cases} \tag{0.476}$$

then we calculate numerically $P(x, t)$ as

$$P\left(x_j, t = t_1\right) \Delta x = \lim_{N \to \infty} \frac{1}{N} \sum_{1}^{N} I\left(x^i\left(t_1\right), \left[x_j, x_j + \Delta x\right)\right) \tag{0.477}$$

for any x_j and various t.

Where $x_j = j\Delta x$ and $j = j_{\min}, j_{\min} + 1, \ldots j_{\max} - 1, j_{\max}$ (uniform mesh). For example, if the process was Brownian, then $P(x, t)$ would be very well approximated by a Gaussian distribution with zero mean and variance t,

as we saw before. Notice that if we say $x_j = x, t = t$, and take the limit $\Delta x \to 0$, then

$$P(x,t) = \lim_{N\to\infty} \frac{1}{N} \sum_i^N \delta\left(x - x_i(t)\right) \text{ as } \lim_{\Delta x\to 0} \frac{I\left(x^i(t), [x, x+\Delta x)\right)}{\Delta x} = \delta\left(x - x_i(t)\right) \tag{0.478}$$

From the theoretical point of view we want to find out an equation for $P(x,t)$ which gives the PDF of the process $x(t)$. If we are interested in the statistics of the process, then $P(x,t)$ gives all the information we need, for we can calculate all averages we want (all moments) (even though it is not guaranteed that from the PDF we can exactly reconstruct the process $x(t)$ pathwise). Actually, we can calculate the average of any "sufficiently regular" function f. Let's assume that f has compact support in $\mathbb{R}$ and is twice-differentiable, namely $f \in C_c^2(\mathbb{R})$. Then we can calculate $\langle f(x(t))\rangle$, average of f over the process. If we are given N indep. realizations of $x(t)$, then as $N \to \infty$

$$= \lim_N \tfrac{1}{N} \textstyle\sum_i^N f\left(x_i(t)\right) = \lim_N \tfrac{1}{N} \sum_i^N \int dx f(x) \delta\left(x - x_i(t)\right) = \int dx f(x) \lim_N \tfrac{1}{N} \sum_i^N \delta\left(x - x_i(t)\right) \overset{\downarrow}{=} \int dx f(x) p(x,t) \tag{0.479}$$

Hence

$$\frac{d}{dt}\langle f(x(t))\rangle \equiv \int \dot{p}(x,t) f(x) dx \tag{0.480}$$

Here $\langle \cdots \rangle$ means that the average of f has to be calculated over the whole set of trajectories of the process $x(t)$. We now discretize the process in time and Taylor-expand the function $f(x)$:

$$f(x(t+\Delta t)) = f(x(t)) + \Delta x f'(x(t)) + \frac{\Delta x^2}{2} f''(x(t)) + \text{ h.o.t.} \tag{0.481}$$

where from eq. (1) we get

$$\Delta x \equiv x(t+\Delta t) - x(t) = \mu(x(t),t)\Delta t + \sigma(x(t),t)\Delta B(t) \tag{0.482}$$

Therefore from (6) $\Delta f \equiv f(x(t+\Delta t)) - f(x(t))$

$$\begin{aligned} \Delta f &= f'(\mu\Delta t + \sigma\Delta B) + \frac{1}{2} f''(\mu\Delta t + \sigma\Delta B)^2 + \text{ h.o.t.} \\ &= f'(\mu\Delta t + \sigma\Delta B) + \frac{1}{2} f''\left(\mu^2\Delta t^2 + 2\mu\sigma\Delta t\Delta B + \sigma^2\Delta B^2\right) + \text{ h.o.t.} \end{aligned} \tag{0.483}$$

We now consider the average of each term: a) $\left\langle f'\sigma\Delta B\right\rangle = \left\langle f'\sigma\right\rangle\langle\Delta B\rangle = 0$ (Itô prescription) b) $\left\langle f''\mu\sigma\Delta t\Delta B\right\rangle = \left\langle f''\mu\sigma\right\rangle \Delta t\langle\Delta B\rangle = 0$ c) $\frac{1}{2}\left\langle f''\sigma^2\Delta B^2\right\rangle = \frac{1}{2}\left\langle f''\sigma^2\right\rangle\left\langle\Delta B^2\right\rangle = \frac{1}{2}\left\langle f''\sigma^2\right\rangle\Delta t$ (Itô preser. IMPORTANT!) all remaining terms are $O\left(\Delta t^2\right)$. Therefore eq. (5) can be re-written as limit

$$\lim_{\Delta t\to 0}\left\langle\frac{\Delta f}{\Delta t}\right\rangle = \left\langle f'\mu\right\rangle + \frac{1}{2}\left\langle f''\sigma^2\right\rangle = \int dx p(x,t)\left[f'(x)\mu(x,t) + \frac{1}{2} f''(x)\sigma^2(x,t)\right] \tag{0.484}$$

As $f \in C_c^2(\mathbb{R})$ we can integrate by parts and safely assume that f, f' and $f'' \to 0$ as $|x|$ is large enough. Hence

$$\int dx p(x,t)\mu(x,t)\frac{\partial f}{\partial x} \overset{\downarrow}{=} -\int dx f(x)\frac{\partial}{\partial x}(p\mu) \tag{0.485}$$

twice integrated by parts

$$\int dx p(x,t) \frac{\sigma^2(x,t)}{2} \frac{\partial^2 f}{\partial x^2} = \frac{1}{2} \int dx f(x) \frac{\partial^2}{\partial x^2} \left(\sigma^2(x) p\right) \quad (0.486)$$

and

$$\frac{d}{dt}\langle f(x)\rangle = \int dx f(x) \frac{\partial}{\partial t} p(x,t) \quad (0.487)$$

Thus from eqs. (9) and (10) and because $f \in C_c^2(\mathbb{R})$ but arbitrary we end up with

$$\frac{\partial}{\partial t} p(x,t) = -\frac{\partial}{\partial x}[\mu(x,t)p(x,t)] + \frac{1}{2}\frac{\partial^2}{\partial x^2}\left[\sigma^2(x,t)p(x,t)\right] \quad (0.488)$$

This is the forward Fokker-Planck equation corresponding to the process defined in eq. (1) with the Itô prescription. The FP eq. (11) can be used to derive the propagator of the process $x(t)$; we need just to solve it with the initial condition $P(x,t_0) = \delta(x - x_0)$, namely, this gives the fundamental solution $P(x,t \mid x_0,t_0)$. If we can calculate $P(x,t)$ then we can find all the averages (= statistics) of the process defined by the Langevin eq. (1). Notice that eq. (11) is a deterministic and linear PDE for $p(x,t)$.

Eq. (11) can also be written as

$$\frac{\partial p}{\partial t} = -\frac{\partial J}{\partial x}(x,t) \quad (0.489)$$

$$J(x,t) \equiv \mu(x,t)p(x,t) - \frac{1}{2}\frac{\partial}{\partial x}\sigma(x,t)p(x,t) \quad (0.490)$$

where $J(x,t)$ is the flux at x at time t. This form shows that, if the process $x(t)$ is defined in the domain $D \subseteq \mathbb{R}$, then

$$\frac{\partial}{\partial t}\int_D p(x,t)dx = -\int_D \frac{\partial J}{\partial x} dx = -J|_{x\in\partial D} \quad (0.491)$$

where ∂D is the boundary of D. If there is no "leakage" of probability, then $J|_{x\in\partial D} = 0$ and we can set $\int_D p(x,t)dx = 1$ at any time t (conservation of probability).

Notice that eq. (11) must be equipped with boundary conditions if the process $x(t)$ is defined in given domain $D \subset \mathbb{R}$. For instance, if $D = \mathbb{R}^+$one has to define what happens at $x = 0$ at any time $t > 0$.

* Absorbing boundary conditions require: $p(x,t)\big|_{x\in\partial D} = 0, \forall t$ * Reflecting boundary conditions require: $J(x,t)|_{x\in\partial D} = 0 \quad \forall t$ N.B: these are the correct conditions when $\sigma(x,t)|_{x\in\partial D} > 0 \quad \forall t$

Equilibrium solution of the Fokker-Planck equation

Let us assume that $\mu(x,t) = \mu(x)$ and $\sigma(x,t) = \sigma(x)$ and also that the propagator defined by eq. (11) reaches an equilibrium solution, namely

$$\lim_{t\to\infty} p(x,t \mid x_0,t_0) = p^{st}(x) \quad (0.492)$$

what is the form of $p^{st}(x)$? From. eq. (11) $\partial_t p^{st} = 0$ implies

$$-\frac{\partial}{\partial x}\left(\mu(x)p^{st} - \frac{1}{2}\frac{\partial}{\partial x}\sigma^2(x)p^{st}\right) = 0 \tag{0.493}$$

hence

$$J^{st}(x) = \mu(x)p^{st} - \frac{1}{2}\frac{\partial}{\partial x}\sigma^2(x)p^{st} = \text{ const for any } x\,. \tag{0.494}$$

If there is no current at any point $x \in D$, we obtain the equilibrium solution (with reflecting boundary conditions at ∂D)

$$\mu(x)p^{st}(x) = \frac{1}{2}\frac{\partial}{\partial x}\left(\sigma^2(x)p^{st}(x)\right) \tag{0.495}$$

Since

$$\begin{aligned} &\frac{2\mu}{\sigma^2}\left(\sigma^2 p^{st}\right) = \frac{\partial}{\partial x}\left(\sigma^2 p^{st}\right) \\ &\sigma^2 p^{st} = \text{ const } e^{\int^x \frac{2\mu}{\sigma^2}dy} \end{aligned} \tag{0.496}$$

hence the equilibrium solution has the form (ref.bound. at x_m, x_M)

$$p^{st}(x) = \frac{1}{Z}\frac{1}{\sigma^2(x)}e^{2\int_{x_m}^x \frac{\mu(y)}{\sigma^2(y)}dy} \quad x_m \le x \le x_M \tag{0.497}$$

where $Z \equiv \int_{x_m}^{x_M} \frac{dx}{\sigma^2(x)}e^{2\int_{x_m}^x \frac{\mu(y)}{\sigma^2(y)}dy} < \infty$, and $\int_{x_m}^{x_M} p^{st}(x)dx = 1$. Some caveats: Notice that eq. (13) may not exist. Also we have not proved that it is unique, nor that it can be reached by some initial conditions. Eq. (13) is only the form one expects if indeed an equilibrium solution exists. Indeed, it does not depend on initial conditions and the equilibrium sol. is only determined by μ and σ (and the ref.b.c.), so it is an intrinsic property of the system which is not tuned by how we initially prepare the system.

The Ornstein-Uhlenbeck process

As a simple application of what we have studied we investigate the O.-U. process. From previous lectures we know that it is defined by the SDE

$$\begin{cases} dx = -\mu x dt + \sigma dB(t) & \text{or} \quad \dot{x} = -\mu x + \sigma\xi_t \\ x(0) = x_0 & (\langle\xi_t\rangle = 0, \langle\xi_t\xi_{t'}\rangle = \delta(t-t')) \end{cases} \tag{0.498}$$

Where μ, σ are positive constants and B is the B.m. From e. (11) we obtain the F.P. equation for the PDF:

$$\dot{p} = -\frac{\partial}{\partial x}[(-\mu x)p] + \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}p \tag{0.499}$$

The equilibrium distribution of (15) (from eq. (13)) is

$$p^{st}(x) \propto e^{-\frac{2}{\sigma^2}\int^x \mu y dy} = e^{-\frac{\mu}{\sigma^2}x^2} \tag{0.500}$$

$$p^{st}(x) = \sqrt{\frac{\mu}{\pi\sigma^2}}e^{-\frac{\mu}{\sigma^2}x^2} \tag{0.501}$$

which is a Gaussian distribution with mean 0 and variance $\frac{\sigma^2}{2\mu}$. Exercise: Show that the equation for the variance that one gets from eq. (14) is the same that one gets from eq. (15). Verify that at stationarity the value is $\sigma^2/2\mu$.

Indeed one can calculate the evolution in time of the PDF.

By taking the Fourier transform of eq. (15) (which gives you the time evolution of the characteristic function of the process) one finds the full solution (which is the propagator of the O.-U. process)

$$\mathrm{p}(x,t \mid x_0,s) = \sqrt{\frac{\mu}{\pi\sigma^2\left(1-e^{-\mu(t-s)}\right)}}\, e^{-\frac{\mu}{\sigma^2}\frac{\left(x-x_0e^{-\mu(t-s)}\right)^2}{1-e^{-\mu(t-s)}}} \tag{0.502}$$

for which $P\left(x,s \mid x_0,s\right) = \delta\left(x-x_0\right)$. Another way to find the solution is to start from the ansatz

$$\mathrm{p(x,\,t)} \propto e^{-Ax^2+xB+C} \tag{0.503}$$

sub this into eq. (15) and find A, B and C as a function of t and x_0. The normalization and the initial condition finally give eq.(17).

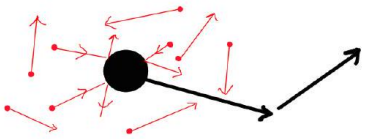
All these findings can be generalized to the case

$$=\text{-}\partial \frac{}{\partial x[(\alpha-\mu x)p]+\frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2}p} \tag{0.504}$$

and also to the multidimensional O.-U. process (Gardiner, p. 105).

Particle in a large medium

We study the motion of a particle suspended in a large (fluid) medium. The particle should be much bigger than those of the medium but small enough to change position and momentum when colliding with the medium's particles. The surrounding medium is a heat bath at thermal equilibrium with a const. temperature T (homogeneous and isotropic). If we had to account for all interactions of the suspended (mesoscopic) particle of mass m, we would write * Fluid particles at temp T * mesoscopic



particle

$$\mathrm{m\ (t)}=_{\mathrm{ext}}\left(\vec{x}(t)\right) + \sum_i^N i\vec{F}\left(\vec{x}(t)-\vec{x}_i(t)\right) \tag{0.505}$$

where $\vec{F}_{\mathrm{ext}}$ is an external force that may (or not) be described by a potential, where the i-th particle exerts on susp. particle a force $\vec{F}\left(\bar{x}-\overline{x_i}\right)$. As $N \simeq N_A$ (Avogadro number), it is pointless to integrate eq. (18). It's more appropriate to treat the medium particles in an effective way, like an effective force acting on the susp. particle. Thus

$$\sum_i^N i\vec{F}\left(\vec{x}(t)-\vec{x}_i(t)\right) \simeq \vec{F}_{\mathrm{aver}} + \vec{F}_{\mathrm{noise}} \tag{0.506}$$

As the mesoscopic particle collides with the smaller fluid particles there is viscous damping generated by the collisions in the fluid. If the velocity of the particle isn't too large we can approximate $\vec{F}_{\text{aver}} = -\gamma\vec{v} = -\gamma\dot{\vec{x}}$, γ being the damping coefficient. From hydrodynamics, we can set $\gamma = 6\pi\eta R$, η being the viscosity and R the Brownian particle's radius. We also assume that all fluid particles have independent motions and every particle's movement is independent on different time intervals (if not too small).

Also, if there is a time interval τ (much smaller of time intervals of observation Δt) large enough that in any two successive time intervals τ the motions of the mesoscopic particle can be considered independent events, then we can effectively approximate $\vec{F}_{\text{noise}}$ as a stochastic process that is proportional to a Brownian motion. For simplicity, let's consider the 1-d case with no external forces. So from (18)

$$\text{m} = -\gamma\dot{x} + \sigma\xi(t) \tag{0.507}$$

where $\langle\xi\rangle = 0$ and $\langle\xi(t)\xi(t')\rangle = \delta(t-t')$. Notice that this process is non-Markovian. Let's multiply both sides by x, then

$$\text{m x d}\overline{\dot{x}=-\gamma x\dot{x}+\sigma x\xi_t} \tag{0.508}$$

Since $\frac{d^2}{dt^2}x^2 = 2\left(\dot{x}^2 + x\ddot{x}\right)$, then

$$\text{m}\overline{2\frac{d^2}{dt^2}(x^2)-m\dot{x}^2=-\frac{\gamma}{2}\frac{d}{dt}(x^2)+\sigma x\xi_t} \tag{0.509}$$

Take the average of both sides and use Itô prescription:

$$\text{m}\overline{2\frac{d^2}{dt^2}\langle x^2\rangle-m\langle\dot{x}^2\rangle=-\frac{\gamma}{2}\frac{d}{dt}\langle x^2\rangle} \tag{0.510}$$

Because of the equipartition theorem in classical mechanics

$$\text{m}\overline{2\langle\dot{x}^2\rangle=\frac{1}{2}k_BT} \tag{0.511}$$

k_B : Boltzmann's constant hence T: absolute temperature

$$\text{m d}^2\overline{dt^2\langle x^2\rangle+\gamma\frac{d}{dt}\langle x^2\rangle=2k_BT} \tag{0.512}$$

Define $y(t) = \frac{d}{dt}\left\langle x^2\right\rangle$, then (19b) becomes

$$\text{m} + \gamma y = 2k_BT \tag{0.513}$$

Whose solution is y(t)=c $\text{e}^{-\frac{\gamma}{m}t} + \frac{2k_BT}{\gamma}$ and c is an arbitrary constant. In suspended particles $\frac{m}{\gamma} \simeq 10^{-8}$sec, which on temporal scales of observation is a tiny time. Hence for $t \gg 10^{-8}$sec, $y \simeq \frac{2k_BT}{\gamma}$ and

$$\text{d}\overline{dt\langle x^2\rangle\simeq\frac{2k_BT}{\gamma}} \tag{0.514}$$

so

$$\left\langle x^2(t)\right\rangle - \left\langle x_0^2\right\rangle = \frac{2k_BT}{\gamma}t \text{ for } t \gg 10^{-8}\text{sec} \tag{0.515}$$

linear increase of the mean square deviation. This reminds us of the

simple Brownian motion. Indeed, let's start from

$$=\sqrt{2D}\xi_t \text{ or } dx = \sqrt{2D}dB(t) \tag{0.516}$$

which leads to the diffusive equation

$$\partial \underbrace{\partial t p(x,t)=D\frac{\partial^2}{\partial x^2}p(x,t) \quad D \text{ is diffusivity}} \tag{0.517}$$

From (21) $x(t) = x_0 + \sqrt{2D}B(t)$ and

$$\left\langle x^2 \right\rangle = \left\langle x_0^2 + 2x_0\sqrt{2D}B(t) + 2DB(t)^2 \right\rangle = x_0^2 + 2Dt \tag{0.518}$$

diffusion law

By comparing eq. (20) and (22), we obtain

$$\mathrm{D}=\mathrm{k}_B T\frac{}{\gamma} \tag{0.519}$$

Einstein's relation

This is the first and simplest example of fluctuation-dissipation theorem.

Obs:

* Eq. (23) tells how we should choose the diffusivity if we want to interpret physically the mesoscopic particle as a free particle within an equilibrium thermal bath at temper. T. * D does not depend on initial conditions, or the nature of interactions between the fluid particles and the Brownian particle, all we need to know is that the system is at equilibrium in a system where general behavior is summarized by the damping constant γ. (We captured some universal behavior here!). * From the diffusion law in eq. (22) one can measure D, hence we can give an estimate of k_B and $N_A = \frac{R}{k_B}$, the Avogadro number (R is the gas constant). This is what Einstein suggested in his 1905 pioneering work on Brownian motion. * This interpretation is straightforward if we start from eq. (19) with $\sigma = \sqrt{2\gamma k_B T}$ and then take the limit $\frac{m}{\gamma} \to 0$ which is called the overdamped limit:

$$\mathrm{m}\underbrace{\gamma\ddot{x}=-\dot{x}+\frac{\sqrt{2\gamma k_B T}}{\gamma}\xi_t \xrightarrow{m/\gamma\to 0} \quad \dot{x}=\sqrt{2\frac{k_B T}{\gamma}}\xi_t} \tag{0.520}$$

overdamped Langevin equation

Connection with Statistical Mechanics

From stat. Mech. we know how to calculate the PDF that a particle has momentum $\vec{p}$ and position $\vec{x}$ when it is located within an external potential $U(\vec{x})$ and is surrounded by a heat bath at equilibrium at temperature T. This is

$$\mathbb{P}(\vec{x},\vec{p}) = \frac{1}{z}e^{-\beta\left(\frac{\vec{p}^2}{2m}+U(\vec{x})\right)} \quad \begin{matrix}\text{Boltzmann's weight} \\ \beta = \dfrac{1}{k_B T}\end{matrix} \tag{0.521}$$

where m is the mass of the particle, $z = \int d\vec{p} \int d\vec{x} \mathbb{P}(\bar{x}, \bar{p}) = (2\pi m k_B)^{3/2} z_0$ is the total partition function and z_0 the reduced one. From eq. (24) one gets the PDF to observe the particle at $\vec{x}$ at equilibrium regardless of its momentum. This is

$$\text{w()=1}\overline{z_0 e^{-\beta U(\vec{x})}} \tag{0.522}$$

Can we connect these classical results with the theory we have developed so far? Yes! We will do it for a 1-d system, but the generalization is simple and direct. Let's start from eq. (19) where now we assume that the particle experiences a conservative external force $f_{\text{ext}} = -\partial_x U(x)$, being $U(x)$ the potential of the force. We also assume that the Brownian particle is at equil. with the heat bath at temper. T, so $\sigma = \sqrt{2\gamma k_B T}$:

$$\text{m =-}\partial_x U(x) - \gamma \dot{x} + \sqrt{2\gamma k_B T}\xi_t \tag{0.523}$$

In the overdamped limit ($\frac{m}{\gamma} \to 0$) we get

$$\text{=-}\partial_x U \overline{\gamma + \sqrt{2D}\xi_t \quad D=\frac{k_B T}{\gamma}} \tag{0.524}$$

or

$$\text{d x=-1}\overline{\gamma \partial_x U dt + \sqrt{2D} dB(t)} \tag{0.525}$$

The corresponding Fokker-Planck equation of eq. (27) is

$$\partial \overline{\partial t p(x,t) = -\frac{\partial}{\partial x}\left[-\frac{1}{\gamma}(\partial_x U)p\right] + D\frac{\partial^2}{\partial x^2}p} \tag{0.526}$$

You can check that the equilibrium distribution of eq. (28) is given by (see eq eq eq. (13))

$$\text{P}_{\text{eq}}(x) \propto e^{-\frac{1}{D\gamma}\int^x \partial_y U(y) dy} \propto e^{-\frac{1}{D\gamma}U(x)} \tag{0.527}$$

but $D\gamma = k_B T$, so $P_{\text{eq}}(x)$ and $w(x)$ in eq. (25) are exactly the same.

Obs:

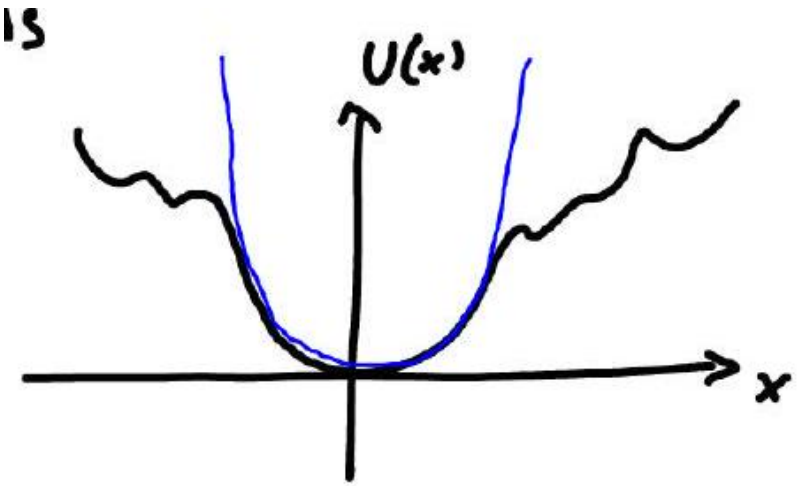
* Notice that we could have fixed $D = \frac{k_B T}{\gamma}$ by imposing that eq eq eq. (29) and (25) are the same! This is remarkable and shows that the value of D does not depend on the potential U, which is somehow unexpected and confirms the universality of Einstein's relation in eq. (23). * Notice that if $U(x) = \frac{1}{2}kx^2$, then eq. (27) reads

$$\text{d x=-k}\overline{\gamma x dt + \sqrt{2\frac{k_B T}{\gamma}} dB(t)} \tag{0.528}$$

which is an O.-U. process with the equilibrium distribution:

$$\text{p}_{\text{eq}}(x) = \sqrt{\frac{k\beta}{2\pi}} e^{-\frac{1}{2}\beta k x^2} \tag{0.529}$$

Brownian particle in contact with a heat bath at equilibrium and forced by a harmonic potential. We start from eq. (26) where $U(x) = \frac{1}{2}kx^2$ and



$\sigma = \sqrt{2\gamma k_B T}$:

$$\text{m =-k x-}\gamma\dot{x} + \sqrt{2\gamma k_B T}\xi_t \tag{0.530}$$

where x is the particle coordinate at time t, m its mass, γ the friction coefficient as before. Eq. (30) is a linear eq. and can be solved even though the process is non-Markovian because of $\ddot{x}$. We write

$$\text{x(t)=x}_c(t) + x_\xi(t) \tag{0.531}$$

where x_c satisfies the homogeneous eq.($\xi = 0$) with $x_c(0) = x_0$ and $\dot{x}_c = v_0$. x_ξ satisfies the in-homog. eq. with $x_\xi(0) = 0$ and $\dot{x}_\xi(0) = 0$. Show that

$$\text{x}_c(t) = Ae^{-\gamma_0 t}\sin(\Omega t) + Be^{-\gamma_0 t}\cos(\Omega t) \tag{0.532}$$

where A, B are arbitrary constants and

$$\gamma_0 = \frac{\gamma}{2m}, \quad \Omega = \omega_0^2 - \gamma_0^2, \quad \omega_0^2 = \frac{k}{m}; \tag{0.533}$$

and

$$\text{x}_\xi(t) = \sqrt{2\gamma k_B T}\frac{1}{m\Omega}\int_0^t e^{-\gamma_0(t-s)}\sinh[\Omega(t-s)]\xi(s)ds \tag{0.534}$$

Prove that

$$\left\langle x^2(t)\right\rangle = \frac{2\gamma k_B T}{m^2\Omega^2}\int_0^t e^{-2\gamma_0(t-s)}\sinh^2[\Omega(t-s)]ds \underset{t\to\infty}{\longrightarrow} \frac{k_B T}{m\omega_0^2} \tag{0.535}$$

* Can you interpret this result from the physical point of view? * Repeat the calculations for the velocity $v(t) = \dot{x}$ * Can you calculate $\langle x(t)x(s)\rangle$? If necessary, fix $|t-s|$ and take the limit $t \to \infty, s \to \infty$.

Laplace method continued **First Semester**

Lecture 15

Date: 2025-10-10 Profesor: Azaele Sandro

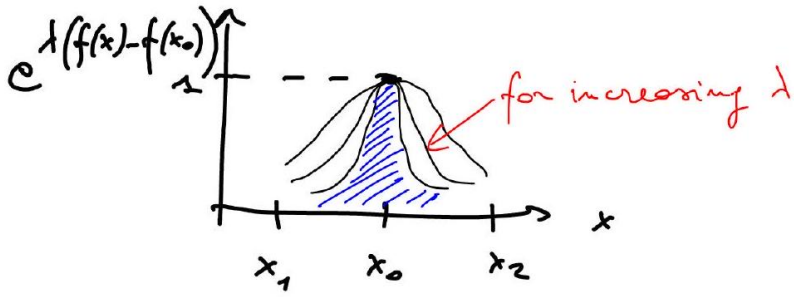
0.16 Laplace method continued

The Laplace method

In several situations we wish to evaluate complicated integrals which have a form

$$I(\lambda) = \int_{x_1}^{x_2} dx g(x) e^{\lambda f(x)} \quad \lambda \in \mathbb{R} \tag{0.536}$$

where g and f are continuous and differentiable functions. Although $I(\lambda)$ cannot be calculated for any arbitrary λ, it happens that it can be well approximated (under appropriate conditions) as $\lambda \to \infty$. The core idea of Laplace's method is that the major contribution to the integral in (21) as $\lambda \to \infty$ comes from the neighborhood of the point in $[x_1, x_2]$ where $f(x)$ gets its maximum value, which we call x_0.



There are essentially three cases:

1. x_0 is an interior maximum, $x_1 < x_0 < x_2$ and $f'(x_0) = 0$. We assume that $f''(x_0) < 0$ (actually if $f'(x_0) = f''(x_0) = f'''(x_0) = 0$ but $f^{(iv)}(x_0) < 0$ we can apply very similar ideas and the calculations are not more difficult). Also $g(x_0) \neq 0$ and it is finite.

As we expect that the dominant contributions comes from the neighborhood of x_0 and $f(x) = f(x_0) + \frac{(x-x_0)^2}{2} f''(x_0) + O\left(|x - x_0|^3\right)$ as $x \to x_0$, we obtain

$$I(\lambda) \cong \int_{x_1}^{x_2} g(x) e^{\lambda\left(f(x_0) + \frac{(x-x_0)^2}{2} f''(x_0)\right)} dx \simeq g(x_0)\, e^{\lambda f(x_0)} \int_{x_1}^{x_2} e^{-\lambda \frac{|f''(x_0)|}{2}(x-x_0)^2} dx \tag{0.537}$$

We change var. $s = (x - x_0)\sqrt{\frac{|f''(x_0)|}{2}\lambda}$ so

$$I(\lambda) \simeq g(x_0)\, e^{\lambda f(x_0)} \sqrt{\frac{2}{\lambda |f''(x_0)|}} \int_{(x_1-x_0)\sqrt{\frac{|f''(x_0)|\lambda}{2}}}^{(x_2-x_0)\sqrt{\frac{|f''(x_0)|\lambda}{2}}} e^{-s^2} ds \tag{0.538}$$

as $\lambda \to \infty \to \int_{-\infty}^{+\infty} e^{-s^2} ds = \sqrt{\pi}$

$$I(\lambda) \simeq g(x_0)\, e^{\lambda f(x_0)} \sqrt{\frac{2\pi}{\lambda |f''(x_0)|}} \quad \text{as } \lambda \to +\infty \text{ (leading order)} \tag{0.539}$$

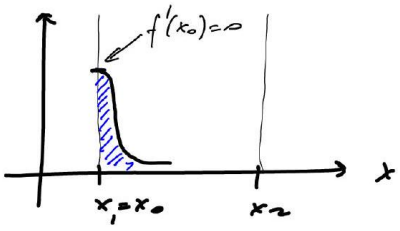
one should prove that this is the leading order (we did not).

Exercise: show that the next to leading order of $I(\lambda)$ in eq. (22) is given by

$$I(\lambda) = e^{\lambda f(x_0)} \sqrt{\frac{2\pi}{\lambda \left| f''(x_0) \right|}} \left(g(x_0) + \frac{c}{\lambda} \right) \quad \text{as } \lambda \to \infty \tag{0.540}$$

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

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



It is easy to show that the leading order formula is

$$I(\lambda) \simeq g(x_0)\, e^{\lambda f(x_0)} \sqrt{\frac{\pi}{2\lambda \left| f''(x_0) \right|}} \tag{0.541}$$

Example

The modified Bessel function of second kind is a special function that occurs in many applications. It is given by

$$K_\nu(x) = \int_0^\infty e^{-x \cosh t} \cosh(\nu t) dt\,, x > 0 \tag{0.542}$$

we wish to estimate $K_\nu(x)$ as $x \to +\infty$ for fixed ν. Since $\cosh'(t) = \sinh(t) > 0$ for $t > 0$, the max of $e^{-x \cosh t}$ as a function of $t (x > 0)$ occurs at $t = 0$, with zero derivative.

So we can apply eq. (23) ($\cosh t \simeq 1 + \frac{t^2}{2} + \cdots$) $f(t) = -\cosh t$

$$K_\nu(x) \simeq e^{-x} \sqrt{\frac{\pi}{2x}} \tag{0.543}$$

as $x \to \infty$ at leading order.

Notice that it does not depend on ν! Exercise: show that

$$K_\nu(x) = \sqrt{\frac{\pi}{2x}} e^{-x} \left(1 + \frac{c(\nu)}{x} + \cdots \right) \tag{0.544}$$

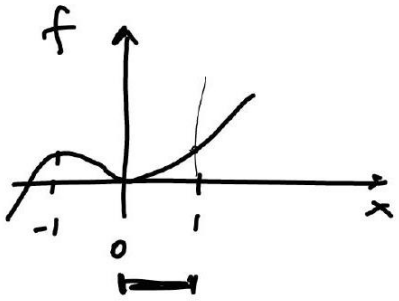
and $c(\nu) = \frac{4\nu^2 - 1}{8}$.

3. $x_0 = x_1$ or $x_0 = x_2$ (x_0 is an endpoint) but $f'(x_0) \neq 0$. Without loss of generality we take $x_0 = x_1$ and $f'(x_0) < 0$.

Example:

Obtain the leading order approximation of

$$\int \mathrm{d}\, x \quad \text{as } \lambda \to \infty \tag{0.547}$$



The max is at $x = 1, f(1) = 5, f'(1) = 12, g(1) = 1$. We can apply eq. (24)

$$I(\lambda) \simeq \frac{e^{5\lambda}}{12\lambda} \tag{0.548}$$

Exercise:

Calculate the leading order approx. when the integral is

$$\int_{-1}^{0} \cdots = ? \quad \int_{-2}^{0} \cdots = ? \tag{0.549}$$

Stirling formula

We want to estimate how fast $N!$ goes to infinity as $N \to \infty$. We will apply the Laplace's method to the gamma function:

$$\Gamma(\lambda) = \int_0^\infty x^{\lambda-1} e^{-x} dx \quad \lambda > 0 \tag{0.550}$$

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

Let's consider $\Gamma(\lambda+1) = \int_0^\infty x^\lambda e^{-x} dx$. If we write this as $\int_0^\infty e^{-x} e^{\lambda \ln x} dx$ we cannot apply Laplace's method. It is more beneficial to consider the max of the function $f(x) = -x + \lambda \ln x$ and set $g(x) = 1$. The max occurs at $x = \lambda$ which suggests a change of var: $x = \lambda t$ (so the max is now fixed w.r.t. t). We get

$$\Gamma(\lambda+1) = \int_0^\infty x^\lambda e^{-x} dx = \lambda^{\lambda+1} \int_0^\infty t^\lambda e^{-\lambda t} dt \tag{0.551}$$

$t^\lambda e^{-\lambda t} = e^{\lambda(\ln t - t)}$ $h(t) = \ln t - t, \quad h'(1) = 0, h''(1) = -1$. In this way we can apply eq. (22) with $g(t) = 1 \quad (t_0 = 1)$.

$$\Gamma(\lambda + 1) = \lambda! \simeq \lambda^{\lambda+1} e^{-\lambda} \sqrt{\frac{2\pi}{\lambda}} \quad \text{as } \lambda \to \infty \tag{0.552}$$

Exercise: Show that at leading order

$$\int_0^\infty e^{-\lambda t} e^{-\frac{1}{t}} dt \cong \frac{\sqrt{\pi} e^{-2\sqrt{\lambda}}}{\lambda^{3/4}} \quad \text{as } \lambda \to \infty \tag{0.553}$$

Example:

Let's consider the class of integrals:

$$I_m(x) = \int_0^\infty t^m e^{-\frac{t^2}{2} - \frac{x}{t}} dt \quad x > 0. \tag{0.554}$$

We calculate $I_m(x)$ for large x and fixed m. $\frac{t^2}{2} + \frac{x}{t}$ has a movable min at $\frac{d}{dt}\left(\frac{t^2}{2} + \frac{x}{t}\right) = 0, \bar{t} = x^{1/3}$. So we introduce the new variable τ:

$$t = x^{1/3}\tau \tag{0.555}$$

So

$$I_m(x) = x^{\frac{m+1}{3}} \int_0^\infty \tau^m e^{-x^{2/3}\left(\frac{\tau^2}{2} + \frac{1}{\tau}\right)} d\tau \tag{0.556}$$

The min of the exponent occurs at $\tau = 1$ (interior) so we can apply eq. (22):

$$\begin{aligned} I_m(x) &= x^{\frac{m+1}{3}} e^{-\frac{3}{2}x^{2/3}} \sqrt{\frac{2\pi}{x^{2/3} \cdot 3}} \\ &= x^{m/3} e^{-\frac{3}{2}x^{2/3}} \sqrt{\frac{2\pi}{3}} \end{aligned} \tag{0.557}$$

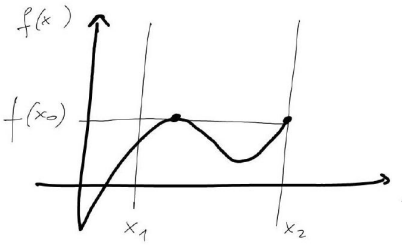
as $x \to \infty$. leading order, fixed m

Exercises:

d t (0.558) $\frac{5\lambda+1}{12\lambda}$

$\int_0^1 \sqrt{1+t}\, e^{\lambda 2t - t^2}$ d t $\simeq$ (0.559) $\sqrt{\frac{\pi}{2\lambda}}$

$\int_{-1}^2 e^{\lambda t^3 - 1}\left(1 + t^2\right) dt \simeq \frac{5e^{7\lambda}}{11\lambda}$ Question: Let's assume that $f(x)$ behaves like in the fig:



Where does the leading order come from?