Lecture Notes on Stochastic Processes

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November 2, 2021

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1 Prerequisites: Probability Theory

1.1 Mathematical Foundations

Probability is a concept based on an idealization, namely the idea of a random experiment. An *ideal random experiment* can be repeated indefinitely often; for each realization, the outcome is unpredictable, but each specific outcome occurs with a constant relative frequency, the *probability* of this outcome. Examples include tossing a fair coin or a perfect dice. Usually, real physical experiments can only be approximated as random experiments, but this approximation is nonetheless surprisingly useful, see Sec. **??**. In mathematics, an axiomatic definition of probability ignores these nuances and just gives the necessary calculation rules.

> **Concept: Probability**
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> Let X be a set of outcomes of a random experiment, then we have the following axioms of probability:
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> 1. $P(A)$ is a function with $0 \leq P(A) \leq 1$ defined for every 'nice' subset $A \subseteq X$
> 2. Additivity: $P(A) + P(B) = P(A \cup B) + P(A \cap B)$
> 3. Normalization: $P(X) = 1$

*Example*1: For a fair coin, the set of possible outcomes is $X = \{\text{head}, \text{tail}\}$ with $P(\{\text{head}\}) = P(\{\text{tail}\}) = 1/2$. (We will often use sloppy notation $p(\text{head})$ for sets A with only single element.)
*Example*2: Perfect dice: $X = \{1, 2, 3, 4, 5, 6\}$, $P(\{1, 2\}) = P(1) + P(2) = 1/3$

Remark: The above axioms apply to 'nice' subsets $A \subset X$. If X is a finite set, all subsets are 'nice'; only if X is uncountably infinite (like the set of real numbers $\mathbb{R}$), there are subsets that are too 'wild' and need to be excluded.

> **Independent random variables**
>
> Suppose a first random experiment yields a random outcome $x_1 \in X_1$ from a set of possible outcomes X_1, while a second experiment yields $x_2 \in X_2$ from a second set of possible outcomes X_2. We can combine these into a single random variable $x = (x_1, x_2)$ that takes values in the product set $X = X_1 \times X_2$ and consider the probability $P(A)$ defined on subsets $A \subseteq X$. The probability $P(x_1)$ of x_1 is then given by the *marginal* probability $P(x_1) = P(\{x_1\} \times X_2)$, i.e., the probability of the

set of all $x = (x_1, x_2)$, where the first component has the definite value x_1 and the second component x_2 is arbitrary. The probability $P(x_2)$ of x_2 is defined analogously. We say the random variables x_1 and x_2 are *independent* if and only if

$$P(x_1, x_2) = P(x_1)P(x_2) \quad . \tag{1.1}$$

Example: Two subsequent tosses of an ideal coin are independent. A counter-example would be represented by drawing from an urn without replacement: the first drawing changes the probabilities for the second drawing.

Exercise: For finite X (in fact, countable X), the expectation value is defined as $\langle x \rangle = \sum_{x \in X} xP(x)$. Show that $\langle x_1 x_2 \rangle = \langle x_1 \rangle \langle x_2 \rangle$ for independent random variables x_1 and x_2. Find a counter-example if x_1 and x_2 are not independent.

If $X = \mathbb{R}$ (real numbers), we can consider a *probability density* as a function $p(x) : \mathbb{R} \to \mathbb{R}^+$, which relates to the probability by

$$P(A) = \int_A \mathrm{d}x\, p(x) \tag{1.2}$$

for $A \subseteq \mathbb{R}$.

Remark: Note that $p(x)$ is also called *probability density function* and sometimes written as $\mathrm{PDF}(x) = p(x)$. Also, note the physical units: if, for example, x has units of a length, $[x] = \mathrm{m}$, then the probability density $p(x)$ has units of an inverse length, $[p] = \mathrm{m}^{-1}$. Knowing the physical units is extremely useful as it allows to tell apart different objects.

Remark: As a mathematical caveat, Eq. (1.2) cannot be defined for arbitrarily "wild" sub-sets $A \subset \mathbb{R}$, but only for sufficiently 'nice' subsets (similar to the restriction of 'nice' subsets in the axiomatic definition of probability). Specifically, these subsets need to be measurable. In particular, (countable) unions and intersections of intervals are measurable, forming a so-called σ-algebra. This technical issue is extensively studied in the mathematical sub-discipline of Measure and Integration Theory, but usually is not a concern in physical applications. For a reference, see e.g. [**Billingsley2012**].

The *cumulative density function* is defined as

$$\mathrm{CDF}(x) = \int_{-\infty}^{x} \mathrm{d}x'\, p(x') \quad . \tag{1.3}$$

The *expectation value* of a function $f(x)$ with respect to a probability density $p(x)$ is

defined as

$$\langle f(x) \rangle = \int \mathrm{d}x \, f(x) \, p(x) \quad . \tag{1.4}$$

Example: The normalization axiom immediately implies $\langle 1 \rangle = 1$; while $\langle x \rangle$ is the usual mean. More generally, we can define special expectation values known as moments and cumulants, which provide important characteristics of a probability distribution.

Moments

The *moments* of a probability distribution $p(x)$ are defined as

$$\mu_n = \langle x^n \rangle = \int_{-\infty}^{\infty} x^n p(x) \quad . \tag{1.5}$$

The moments μ_n are the Taylor coefficients of the so-called *characteristic function*

$$\langle \exp(tx) \rangle = \sum_{n=0}^{\infty} \mu_n \frac{t^n}{n!} \quad . \tag{1.6}$$

Remark: One may think of the characteristic function as an abstract function that conveniently encodes (almost) all information about a probability distribution $p(x)$ on the real line $\mathbb{R}$.

Remark: For some probability distributions (e.g., probability distributions with polynomial tails, also called 'fat tails'), higher moments may be infinite.

Cumulants

The *cumulants* are given by the mean value $k_1 = \mu_1$, the variance $k_2 = \mu_2 - \mu_1^2$ and higher order cumulants such as $k_3 = \mu_3 - 3\mu_2\mu_1 + 2\mu_1^3$. More generally we have

$$\ln \langle \exp(tx) \rangle = \sum_{n=0}^{\infty} k_n \frac{t^n}{n!} \tag{1.7}$$

Remark: Moments and cumulants contain the same information: To relate cumulants and moments, one can insert Eq. (1.7) into the Taylor series of the exponential function, and collect equal powers of t (after applying the binomial formula to expand powers); thereby, one obtains complicated formulas expressing the nth moment μ_n in terms of all k_k, $k \leq n$. The series of moments "almost" uniquely determines the underlying probability density

function $p(x)$ (yet there are some mathematical delicacies for which we refer the reader to the mathematics literature). Often, moments can be computed more directly, while cumulants allow to read off relevant information more readily.

Example: For the normal distribution (discussed below) $p_{\mathrm{norm}}(x) = (2\pi\sigma^2)^{-1/2} \exp[-(x-\mu)^2/(2\sigma^2)]$ with mean μ and variance σ^2, we have $k_0 = \mu_0 = 1$ (this is just the normalization condition), $k_1 = \mu_1 = \mu$ (mean), $k_2 = \mu_2 - \mu_1^2 = \sigma^2$ (variance), as well as $k_n = 0$ for $n \geq 3$. Conversely, a probability distribution whose higher cumulants vanish, i.e., $k_n = 0$ for $n \geq 3$, is necessarily a normal distribution.

1.2 Probability in Physics

In physics, probability is usually estimated as the *relative frequency* of an outcome A in an experiment that can be repeated indefinetely often with the same initial macrostate: If N_A is the number of realizations of the experiment resulting in A and N the total number of realizations, the probability $P(A)$ of A is estimated as

$$P(A) \approx \frac{N_A}{N} \quad , \tag{1.8}$$

for N sufficient large. (In the case of ideal random experiments, one can show mathematically that this estimate indeed converges to the true probability in the vast majority of cases. Indeed, the probability of large errors converges rapidly to zero for large N, albeit it never becomes exactly zero. We will later specify the expected error of such an estimate.)

Example: The distinction between *macrostate* and *microstate* is important here: Throwing a dice would not be random anymore if we exactly knew its initial position and momentum, i.e., its microstate, because the motion of the dice is deterministic. But since the motion of the dice bouncing on the table is highly chaotic, the outcome is essentially random if the initial microstate is only known approximately, i.e., if we only know the initial macrostate. This is nicely illustrated in a talk entitled "Gott würfelt nicht. Oder doch?" by Jan Nagel [https://youtu.be/q-ezpVF6cL4; in German], which demonstrates how uncertainty in initial conditions leads to effectively stochastic outcomes.

Remark: One may philosophize whether true randomness occurs in quantum systems or not. (The answer depends on which interpretation of quantum mechanics one favors.) Yet, for macroscopic "random experiments", such as tossing a coin or throwing a dice, quantum effects are negligible and the apparent randomness arises solely from chaotic deterministic dynamics and imprecise knowledge of initial conditions.

1.3 Important Probability Distributions

Normal Distribution

Probably the most important probability distribution is the *normal distribution*. If a random variable x is distributed according to a normal distribution with mean μ and variance σ^2, we write $x \sim \mathbb{N}(\mu, \sigma^2)$; the corresponding probability density reads

$$p_{\text{normal}}(x) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left[-\frac{(x-\mu)^2}{2\sigma^2}\right] \quad . \tag{1.9}$$

The moments and cumulants of the normal distribution are given by

$$\mu_1 = \mu,\ \mu_2 = \mu^2 + \sigma^2,\ \mu_3 = \mu^3 + 3\mu\sigma^2$$
$$k_1 = \mu,\ k_2 = \sigma^2,\ k_j = 0 \quad \text{for} \quad j \geq 3 \quad .$$

The cumulative probability distribution function CDF of the normal distribution with mean zero, $\mu = 0$, and unit variance, $\sigma^2 = 1$, has its own name, *error function*, abbreviated (x). The importance of the normal distribution stems from the fact that many other probability distributions can be approximated by a normal distribution in a suitable limit.

Exercise: Compute the characteristic function $\langle \exp(tx) \rangle$ of a normal distribution with $\mu = 0$ and $\sigma^2 = 1$. By taking its logarithm, verify above formulas for the cumulants for this special case. Hint: Start with the definition of the expectation value $\langle \exp(tx) \rangle$ as an integral, combine the exponentials and complete the square in its exponent; the resultant integral is already known.

Binomial Distribution

A Bernoulli trial has two possible outcomes, say "yes" and "no", with respective probabilities p and $1-p$. If we perform n independent trials, the probability to obtain k-times the outcome "yes" is given by the so-called *Binomial distribution*

$$P_{\text{binom}}(k) = \binom{n}{k} p^k (1-p)^{n-k} \quad . \tag{1.10}$$

The proof counts the number $\binom{n}{k}$ of paths in a binary decision tree with exactly k-times "yes", and multiplies this number with the constant probability $p^k(1-p)^{n-k}$ for each of these paths. The mean and variance read $\langle k \rangle = np$ and $\langle k^2 \rangle - \langle k \rangle^2 = np(1-p)$.

In practical applications with large n, one can do a normal approximation by $k \sim \mathcal{N}(np, np(1-p))$.

Poisson Distribution

The Poisson distribution can be regarded as a continuous-time limit of the Binomial distribution. Specifically, we can assign time points $t_j = j\,dt$, $j = 1, \ldots, n$ to the n subsequent Bernoulli trials. We assume that events occur with a constant rate r; the probability that an event occurs in the short time interval dt is then approximately given by $r\,dt$ (more precisely $1 - exp(-r\,dt) = r\,dt + \mathcal{O}((()r\,dt)^2)$.

We take the limit $n \to \infty$, with rate r held constant. Then the total number k of events during the observation time $T = n\,dt$ becomes a random variable that is distributed according to a *Poisson distribution* with parameter $\lambda = r\,T$

$$P_{\text{Poisson}}(k) = \exp(-\lambda)\frac{\lambda^k}{k!} \quad . \tag{1.11}$$

Here, λ represents the expected number of events during the observation time $T = n\,dt$.

Exercise: Read about Stirling's formula and then prove Eq. (1.11) as a limit of the Binomial distribution.

Now take the limit $n \to \infty$ with $\lambda = \text{const}$ and $p = \frac{\lambda}{n}$, so we get the Poisson distribution with $\mu = \langle k \rangle = \lambda$, $\sigma^2 = \langle k^2 \rangle - \langle k \rangle^2 = \lambda$. An approximation is $p(k, \lambda) = N(\lambda, \lambda)$, valid for very large λ.

Remark: Why is the concept of time being used here?

The Poisson distribution is an example of a stochastic Poisson process

$$f(t) = \sum_{-\infty}^{\infty} \delta(t - t_j) \tag{1.12}$$

and so $k = \int_0^T f(t)$.

Examples of Poisson-distributed random variables are the number of radioactive decay events in a given time interval, or photons arriving at a CCD sensor. Similarly, the number of service requests submitted to a computer server follows a Poisson distribution, which has practical applications in queuing theory.

Power-law distribution

Finally, some have so-called "fat tails", i.e.,

$$p(x) \sim x^{-\alpha} \quad \text{for} \quad x \gg 1 \quad . \tag{1.13}$$

Examples of such *power-law distributions* include the distribution of Facebook contacts (where $\alpha = 2.2$), or the distribution of jumps in idealized models of animals foraging for food (Lévy walks).

Power-law distributions have some unpleasant mathematical properties, such as a divergent variance $\sigma^2 \to \infty$ for $\alpha < 3$.

1.3.1 Empirical mean and empirical standard deviation

We consider a sequence n of $x_1, ...x_n$ of independent, identically distributed, random variables with mean μ and variance σ^2. (One may think of the same experiment repeated n times under identical conditions.) We define the *empirical mean* by

$$\bar{x} = \frac{1}{n}(x_1 + \cdots + x_n) = \text{empirical mean} \quad , \tag{1.14}$$

and the *empirical variance* by

$$\widehat{\sigma}^2 = \frac{1}{n-1}\left((x_1 - \bar{x})^2 + \cdots + (x_n - x)^2\right) = \text{empirical variance} \quad . \tag{1.15}$$

Of course, $\bar{x}$ and $\widehat{\sigma}^2$ are now themselves random variables.

Obviously,

$$\langle \bar{x} \rangle = \mu \quad , \tag{1.16}$$

i.e., the expectation value of the empirical mean equals the true mean. One says that $\bar{x}$ is *faithful* estimator of μ.

Similarly, for the special case that the x_j are normally distributed, $x_j \sim \mathcal{N}(\mu, \sigma^2)$, we have

$$\langle \widehat{\sigma}^2 \rangle = \sigma^2 \quad , \tag{1.17}$$

i.e., the expectation values of the empirical variance equals the true variance. Even in a general case, where the x_j are not normally distributed, $\widehat{\sigma}^2$ often gives a useful approximation of the true variance.

1.3.2 The Central-Limit Theorem

We present the famous central-limit theorem, which states that the sum of many random variables will be approximately normal distributed. We sketch the idea for its proof based on the convergence of characteristic functions. As an application, the normal approximation for the Bionomial distribution discussed above can be considered a corrolary of the central-limit theorem.

Central-Limit-Theorem

Consider a sequence of $x_1, ...x_n$ of independent, identically distributed, random variables (Bernoulli trials) with mean μ and variance σ^2. We define the empirical mean by

$$\bar{x} = \frac{1}{n}(x_1 + \cdots + x_n) = \text{empirical mean} \tag{1.18}$$

We normalize it to a random variable with expectation value zero

$$z = \frac{\bar{x} - \mu}{\sigma/\sqrt{n}} \quad . \tag{1.19}$$

Then the probability distribution $p(z) \to N(0,1)$ for large n ("convergence in distribution"), or, equivalently, $\text{CDF}(z) \to \text{Erf}(z)$ for almost all $z \in \mathbb{R}$

Idea of proof:

The idea of the proof is to compute the cumulants of x_j

$$k_1 = \mu,\ k_2 = \sigma^2 \ldots \tag{1.20}$$

and then to show that the cumulants of z_j are given by

$$k_1 = 0,\ k_2 = 1,\ k_3 \sim \frac{1}{\sqrt{n}},\ k_4 \sim \frac{1}{n} \ldots \tag{1.21}$$

and

$$\lim_{n\to\infty} \ln\langle zt\rangle = \lim_{n\to\infty} \sum_{l=0}^{\infty} k_l t^l = 1 + \frac{1}{2}t^2 \quad . \tag{1.22}$$

Then we have $p(z) \to N(0,1)$. To show this behavior of the cumulants, we take a look at the function

$$C_x(t) = \exp(\langle xt\rangle) \text{ with } C_{\alpha x}(t) = C_x(\alpha t),\ \alpha \in \mathbb{R} \tag{1.23}$$

which satisfy $\langle(\alpha x)^j\rangle = \alpha^j \langle x^j\rangle$ and $k_{\alpha x,j} = \alpha^j k_{x,j}$ for all cumulants, i.e. $\forall j \in \mathbb{N}$. Use this for $\bar{x}, z$:

$$C_{\bar{x}}(t) = C_{x_1}\left(\frac{t}{n}\right) C_{x_2}\left(\frac{t}{n}\right) \dots C_{x_n}\left(\frac{t}{n}\right) = \left(C\left(\frac{t}{n}\right)\right)^n$$

$$C_z(t) = C_{\bar{x}}\left(\frac{t}{\sigma/\sqrt{n}}\right) \exp\left(-\frac{\mu t}{\sigma/\sqrt{n}}\right) = \left(C_x\left(\frac{t}{\sigma/\sqrt{n}}\right)\right)^n \exp\left(-\frac{\mu t}{\sigma/\sqrt{n}}\right)$$

giving us

$$\ln(C_z(t)) = n \ln\left(C_x\left(\frac{t}{\sigma/\sqrt{n}}\right)\right) - \frac{\mu t}{\sigma/\sqrt{n}} \tag{1.24}$$

and so we get

$$k_{z,j} = n\left(\frac{1}{\sigma\sqrt{n}}\right)^j k_{x,j} \tag{1.25}$$

1.3.3 Normal Approximation

In this section we are going to show, that the Bernoulli distribution

$$p(k,n) = \binom{n}{k} p^k (1-p)^{n-k} \tag{1.26}$$

can be approximated by using a normal distribution

$$p(k,n) \approx \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{(k-np)^2}{2\sigma^2}\right) \tag{1.27}$$

with $\sigma^2 = npq$.

Proof I Using Stirling's Approximation

For this proof we introduce a small deviation ε such that $q = 1 - p$, $k = np + n\varepsilon$ and $p(k,n) \approx 0$ for $\varepsilon \gg \frac{1}{\sqrt{N}}$. The first trick is then to use Stirling's approximation

$$n! \approx \sqrt{2\pi n}\left(\frac{n}{e}\right)^n \tag{1.28}$$

which leads us to

$$\begin{aligned} p(k,n) &= \frac{\sqrt{2\pi n}}{\sqrt{2\pi k}\sqrt{2\pi(n-k)}} \frac{n^n}{k^k(n-k)^{n-k}} p^k q^{n-k} \\ &= \left[\frac{1}{\sqrt{2\pi pqn}} + \mathcal{O}(\varepsilon)\right] \left(\frac{np}{k}\right)^k \left(\frac{nq}{n-k}\right)^{(n-k)} \end{aligned}$$

The second trick is to apply $x^k = \exp(k\ln(x))$, so we need to evaluate the following two expressions

$$\ln\left(\frac{np}{k}\right) = \ln\left(\frac{p}{p-\varepsilon}\right) = -\ln\left(1 + \frac{\varepsilon}{p}\right) \approx -\frac{\varepsilon}{p} + \frac{1}{2}\left(\frac{\varepsilon}{q}\right)^2$$

$$\ln\left(\frac{nq}{n-k}\right) = \ldots \approx \frac{\varepsilon}{p} - \frac{1}{2}\left(\frac{\varepsilon}{q}\right)^2$$

which implies

$$\begin{aligned}\left(\frac{np}{k}\right)^k \left(\frac{nq}{n-k}\right)^{n-k} &\approx \exp\left(k\left[-\frac{\varepsilon}{p}+\frac{1}{2}\left(\frac{\varepsilon}{q}\right)^2\right]+(n-k)\left[\frac{\varepsilon}{p}-\frac{1}{2}\left(\frac{\varepsilon}{q}\right)^2\right]\right)\\ &= 0\cdot\varepsilon-\frac{1}{2}n\frac{\varepsilon^2}{p}-\frac{1}{2}n\frac{\varepsilon^2}{q}+\mathcal{O}(\varepsilon^3)\\ &= -\frac{1}{2}\frac{\varepsilon^2(p+q)}{pq}=-\frac{1}{2}\frac{(k-np)^2}{npq}\end{aligned}$$

Thus,

$$p(k,n)\approx\frac{1}{\sqrt{2\pi\sigma^2}}\exp\left(-\frac{(k-np)^2}{2\sigma^2}\right) \tag{1.29}$$

with $\sigma^2 = npq$.

1.4 Stochastic Processes

Stochastic processes describe the stochastic evolution of a random variable as function of time t. Stochastic processes have applications in physics, e.g., to model the effect of thermal fluctuations, in chemistry, e.g., to model chemical reactions when the number of interacting molecules is small, in biology, e.g., to model population dynamics of cells in a tissue, and finance, e.g., to forcast the variability of stock prices.

Stochastic Process

A stochastic process is a random function $f(t) : \mathbb{R} \to \mathbb{R}$, i.e. a family of random variables parameterized by $t \in \mathbb{R}$.

Terminology

- conditional probability density: $p(f(t_2) = f_2 | f(x_1) = f_1)$
- Markov property: For $t_3 > t_2 > t_1$ it holds that $p(f(t_3) = f_3 | f(x_2) = f_2, f(x_1) = f_1) = p(f(t_3) = f_3 | f(x_2) = f_2)\ \forall t_j, f_j$, example: diffusion, counter-example: random draw from an urn without replacements
- Martingales: Markov processes with the property $\langle f(t_2) | f(t_1) = t_1 \rangle = f_1$, example: diffusion, counter-example: diffusion with drift

Example: Poisson Process

Poisson Process

For a Poisson process, events occur independently with constant rate r at random times t_j

$$f(t) = \sum_{j=-\infty}^{\infty} \delta(t - t_j) \quad . \tag{1.30}$$

We have $\langle f(t) \rangle = r$; moreover $\langle f(t) f(t') \rangle = r^2 + r\delta(t - t')$. The quantity $N = \int_0^T f(t)$ counts the number of events in the finite time interval $[0, T]$, where T is total observation time; this number N follows a Poisson distribution with parameter $\lambda = rt$:

$$P(N = k) = P_{\text{Poiss}}(k, \lambda = rT) \tag{1.31}$$

The waiting times $t = t_{j+1} - t_j$ between subsequent events are exponentially distributed, i.e. $p(t) = r\exp(-rt)$.

The last property can be proven as follows: by taking a look at the *survival probability* $P(t \geq \theta)$, i.e., the probability that no event occured since $t = 0$. CDF, for which we have

$$P(t \geq \theta + \mathrm{d}t) = P(t \geq \theta) - r\,\mathrm{d}t\,P(t \geq \theta)$$

so that

$$\frac{\mathrm{d}}{\mathrm{d}t}P(t \geq \theta) = -r\,\mathrm{d}t\,P(t \geq \theta) \quad \Rightarrow \quad P(t \geq \theta) \sim \exp(-rt) \quad .$$

Note that rdt is dimensionless, thus $rdt \ll 1$ is meaningful.

Example: Gaussian White Noise

Gaussian white noise

Gaussian white noise is a (generalized) function $\xi(t) : \mathbb{R} \to \mathbb{R}$ with the following properties

i) $\langle \xi(t) \rangle = 0$

ii) $\langle \xi(t)\xi(t') \rangle = 2D\delta(t - t')$

iii) $\int_{t_1}^{t_2} \mathrm{d}t\,\xi(t) \sim N(0, 2D[t_2 - t_1])$

Gaussian white noise can be considered as the idealization of thermal random forces, corresponding to the limit of vanishing correlation time, $\tau_c \to 0$.

Remark: Gaussian White Noise and Mathematics

Strictly speaking, ξ itself cannot be defined mathematically. Instead mathematicians define a so-called Wiener process

$$W(t) = \int_0^t \mathrm{d}t'\,\xi(t') \tag{1.32}$$

so that $W(t)$ exists and is continuous with probability 1.

For the example of Brownian motion, which we will consider in the next chapter, Gaussian white noise can be considered an idealization of the random thermal force due to collisions of a colloid with solvent molecules (in the limit of vanishing correlation time $\tau \to 0$).

Numerical Implementation of Gaussian White Noise

Gaussian white noise can be implemented numerically for the stochastic differential equation

$$\dot{x} = f(x,t) + \xi(t) \tag{1.33}$$

in an Euler scheme by sampling $\xi_j = \xi(t_j) \sim N(0, \frac{2D}{dt})$ at discrete time steps $t_j = jdt$, which yields

$$x_{j+1} = x_j + \underbrace{f(x_j,t_j)dt}_{\sim dt} + \underbrace{\xi_j dt}_{\sim\sqrt{dt}} + \mathcal{O}(dt^{3/2}) \tag{1.34}$$

Diffusion Approximation

Many stochastic processes can be mapped approximately to Gaussian white noise.

Consider for example a Poisson process with rate r. The total number of events $N = \int_0^{\Delta t} f(t)$ in the time interval Δt has the moments $\langle N\rangle = r\Delta t$ and $\langle (N - r\Delta t)^2\rangle = r\Delta t$. Thus, we can approximate $f(t) \approx r + \xi(t)$, where $\xi(t)$ is Gaussian white noise with $\langle \xi(t)\rangle = 0$ and $\langle \xi(t)\xi(t')\rangle = r\delta(t-t')$

Overview

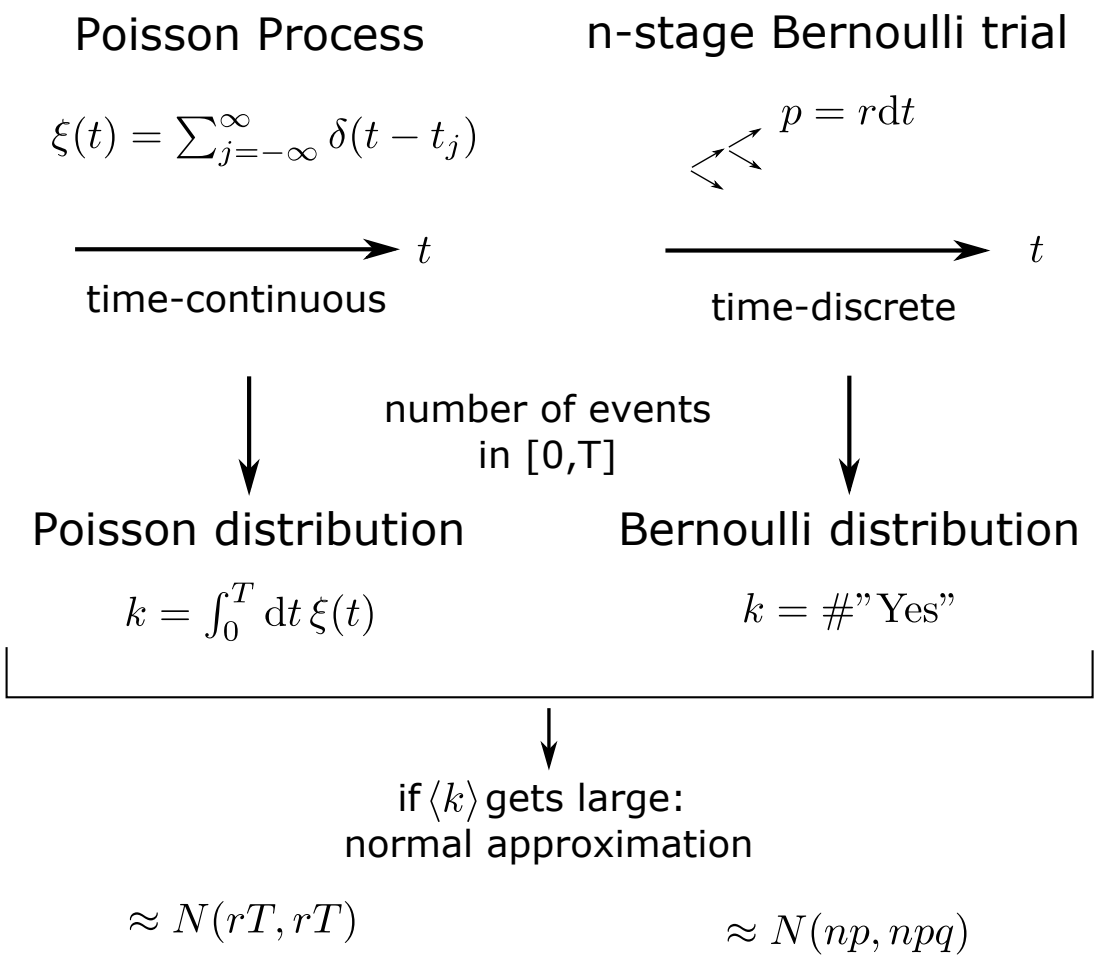


Figure 1.1: Relation between different stochastic processes and their corresponding distributions.

2 Diffusion & Random Walk

2.1 Random Walker

The random walk can be used to model a variety of different phenomena just like

- the motion of a particle during diffusion
- the spread of mosquito infestation in a forest
- propagation of sound waves in a heterogeneous material
- money flow, stock prices

> **Model: Random Walker**
>
> A random walker in d-dimensional space can be considered as a particle moving in steps of length l, while choosing each time a random, uncorrelated direction. Uncorrelated means that
>
> $$\langle \vec{x}_n \cdot \vec{x}_m \rangle = l^2 \delta_{nm}, \quad \vec{x}_n \in \mathbb{R}^d, n \in \mathbb{Z} \tag{2.1}$$
>
> for averaging over the probability distribution of steps $\rho(\vec{x}_n)$.

Thus, the displacement $\vec{x}$ of a random walker after N steps is given by

$$\vec{x} = \sum_{n=1}^{N} \vec{x}_n \quad \text{with} \quad \langle \vec{x} \rangle = \vec{0} \tag{2.2}$$

The mean square displacement $(\Delta\vec{x})^2$ equals the variance σ^2

$$\begin{aligned} \sigma^2 &= \left\langle \vec{x}^2 \right\rangle - \langle \vec{x} \rangle^2 = \left\langle \vec{x}^2 \right\rangle = (\Delta\vec{x})^2 \\ &= \left\langle \left(\sum_{n=1}^{N} \vec{x}_n \right)^2 \right\rangle = \sum_{n,m=1}^{N} \langle \vec{x}_n \cdot \vec{x}_m \rangle = Nl^2 \end{aligned}$$

As we have $(\Delta\vec{x})^2 \sim N$ and $\Delta t \sim N$, the ratio $\frac{(\Delta\vec{x})^2}{\Delta t}$ is a constant in the continuum limit. This is quite unusual since a square term in the numerator appears.

2.2 Continuum Limit: Diffusion Equation

We now consider the step sizes $|\Delta\vec{y}|$ of a random walker becoming infinitesimally small, with $p(\Delta\vec{y})$ being the probability for step $\Delta\vec{y}$:

$$\langle \Delta\vec{y}_i \rangle = \int \mathrm{d}^d \Delta y \, [\Delta y_i \, p(\Delta\vec{y})] = 0 \tag{2.3}$$

$$\langle \Delta\vec{y}_i \, \Delta\vec{y}_j \rangle = \int \mathrm{d}^d \Delta y \, [\Delta y_i \, \Delta y_j \, p(\Delta\vec{y})] = \left\langle (\Delta\vec{y})^2 \right\rangle \frac{\delta_{ij}}{d} \tag{2.4}$$

for $i, j = 1, 2, \ldots, d$ vector components.

We can express the probability for a displacement of $\vec{x}$ after N steps $p_N(\vec{x})$ through the elementary relation

$$P_N(\vec{x}) = \int \mathrm{d}^d \Delta y \, P_{N-1}(\vec{x} - \Delta\vec{y}) P(\Delta\vec{y}) \tag{2.5}$$

Next, we perform a Taylor expansion of $P_N(\vec{x})$

$$\begin{aligned} P_N(\vec{x}) &\approx \int \mathrm{d}^d \Delta y \, P(\Delta\vec{y}) \left[P_{N-1}(\vec{x}) - \Delta y_i \partial_i P_{N-1}(\vec{x}) + \frac{1}{2} \Delta y_i \Delta y_j \partial_i \partial_j P_{N-1}(\vec{x}) \right] \\ &= P_{N-1}(\vec{x}) + \frac{\langle (\Delta\vec{y})^2 \rangle}{2d} \vec{\nabla}^2 P_{N-1}(\vec{x}) \end{aligned}$$

We can define a continuum probability density $p(\vec{x}, t)$ after the time $t = N\Delta t$

$$p(\vec{x}, t) = p(\vec{x}, N\Delta t) := P_N(\vec{x}) \tag{2.6}$$

and now we can take the limit

$$\frac{\partial p}{\partial t} = \lim_{\Delta t \to 0} \frac{P_N(\vec{x}) - P_{N-1}(\vec{x})}{\Delta t} = D \vec{\nabla}^2 p \quad \text{with} \quad D = \frac{\langle (\Delta\vec{y})^2 \rangle}{2d\Delta t} \tag{2.7}$$

This continuum limit exists if D can be treated as a constant, i.e. if $\frac{\langle (\Delta\vec{y})^2 \rangle}{\Delta t}$ is finite for $\Delta t \to 0$. The resulting equation is known as the diffusion equation.

Diffusion Equation

The *diffusion equation* for a probability density $p(\vec{x}, t)$ reads

$$\frac{\partial p(\vec{x}, t)}{\partial t} = D\nabla^2 p(\vec{x}, t) \quad , \tag{2.8}$$

where D is the diffusion coefficient with units $[D] = \mathrm{m}^2\,\mathrm{s}^{-1}$. Alternativly, we can start from the *conservation equation*

$$\frac{\partial p}{\partial t} = -\vec{\nabla} \cdot \vec{J} \tag{2.9}$$

with probability current $\vec{J}$, which reads for the case of the diffusion equation $\vec{J} = -D\vec{\nabla}p$.

Remark: The case of a position-dependent diffusion coefficient $D(\vec{x})$ is somewhat subtle, and requires some microscopic knowledge of the underlying system, see also the section on Ito and Stratonovich calculus.

Solving the diffusion equation

The diffusion equation can be solved e.g. by doing a Fourier transformation of both sides

$$\frac{\partial p}{\partial t} = D\vec{k}^2 p \tag{2.10}$$

leading to the k-space solution

$$p(\vec{k}, t) = \mathcal{F}(p(\vec{x}, t)) = \exp\left(-D\vec{k}^2 t\right) \tag{2.11}$$

A Fourier transform backwards gives the fundamental solution (Green's function)

$$p(\vec{x}, t) = \frac{1}{(4\pi k t)^{d/2}} \exp\left(-\frac{\vec{x}^2}{4kt}\right) \tag{2.12}$$

with the mean square spread $\sigma^2 \sim kt$, which is a spherically symmetric, multivariate normal distribution.

Concept: Diffusion

Diffusion is a net movement of particles from a region of high to a region of low concentration due to random motion of the single particles.

2.3 Random Force Model

Another approach to diffusion is to consider a colloidal particle suspended in a fluid that is experiencing random forces $f(t)$ due to the interaction with the fluid molecules.

Each fluid molecule is governed by the Hamiltonian equations of motion

$$\dot{\vec{p}}_i = -\frac{\partial H}{\partial \vec{q}_i}, \quad \dot{\vec{q}}_i = \frac{\partial H}{\partial \vec{p}_i} \tag{2.13}$$

and their average velocity is characterized by the fluid's temperature T

$$\frac{m}{2}\langle \vec{q}_i^2 \rangle = \frac{k_B T}{2} \tag{2.14}$$

Repetition: Equipartition Theorem

At thermal equilibrium, the system's energy, given by a Hamiltonian H, is distributed on its degrees of freedom x_n via

$$\left\langle x_m \frac{\partial H}{\partial x_n} \right\rangle = \delta_{mn} k_B T \tag{2.15}$$

This holds for a microcanonical and canonical ensemble and relates temperature to the systems average energies.

Model: Random Forces

The motion of a particle under random forces $f(t)$ in one space dimension can be described by Newton's second law via

$$m\ddot{x} + \gamma \dot{x} = f(t) \tag{2.16}$$

where $x(t)$ is the colloid's position and γ is the damping constant.

For long time scales $\tau_m >> \frac{m}{\gamma}$, inertia is negligible and we obtain the overdamped dynamics $\gamma \dot{x} = f(t)$. The random force is characterized through

- $\langle f(t) \rangle = 0$ (by symmetry)

- a vanishing correlation $\langle f(t)f(t+\tau)\rangle \to 0$ for $\tau \gg \tau_m$, with the correlation time τ_m
- stationarity of the random forces:

$$\frac{1}{\gamma^2}\int_{-\infty}^{\infty} \mathrm{d}\tau \, \langle f(t)f(t+\tau)\rangle = 2D \tag{2.17}$$

  with $[D] = \mathrm{m}^2\,\mathrm{s}^{-1}$

In each case the average is taken over the probability distribution of the random force.

Formal Solution

A formal solution to the equation of motion without inertia reads

$$x(t) = x(0) + \frac{1}{\gamma}\int_0^t \mathrm{d}t_1 \, f(t_1) \tag{2.18}$$

Defining $\Delta x := x(t) - x(0)$, we get by symmetry for the mean displacement

$$\langle \Delta x(t)\rangle = \frac{1}{\gamma}\int_0^t \mathrm{d}t_1 \, \langle f(t_1)\rangle = 0 \tag{2.19}$$

and for the mean square displacement

$$\begin{aligned}
\langle \Delta x^2\rangle &= \frac{1}{\gamma^2}\left\langle \left(\int_0^t \mathrm{d}t_1 \, f(t_1)\right)\left(\int_0^t \mathrm{d}t_2 \, f(t_2)\right)\right\rangle \\
&= \frac{1}{\gamma^2}\int_0^t \mathrm{d}t_1 \int_0^t \mathrm{d}t_2 \, \langle f(t_1)f(t_2)\rangle \\
&= \frac{1}{\gamma^2}\int_0^t \mathrm{d}t_1 \int_{-t_1}^{t+t_1} \mathrm{d}\tau \, \langle f(t_1)f(t_1+\tau)\rangle \\
&= \frac{1}{\gamma^2}\int_0^t \mathrm{d}t_1 \int_{-\infty}^{\infty} \mathrm{d}\tau \, \langle f(t_1)f(t_1+\tau)\rangle + \mathcal{O}(D\tau_m) \\
&= \frac{1}{\gamma^2}\int_0^t \mathrm{d}t_1 \, \gamma^2 2D = 2Dt
\end{aligned}$$

Calculating $D = D(T)$

In order to calculate $D(T)$, we do a trick and add an elastic spring to the model

$$kx + \gamma\dot{x} = f(t) \tag{2.20}$$

So at first we might ask what happens in reaction to a pulse response?

$$kx + \gamma\dot{x} = \rho_0\delta(t) \quad \text{with} \quad x(t) = 0\,|\,t < 0 \tag{2.21}$$

The solution to this scenario is given by

$$x(t) = \rho_0\chi(t), \quad \chi(t) = \frac{1}{\gamma}\exp\left(-\frac{t}{\sigma}\right)\Theta(t), \quad \sigma = \frac{\gamma}{k} \tag{2.22}$$

We get back to the full problem, where the formal solutions reads

$$x(t) = \int_0^\infty \mathrm{d}\tau\, f(t-\tau)\chi(\tau) \tag{2.23}$$

with $\langle x(t)\rangle = 0$ by symmetry and

$$\begin{aligned}
\langle \Delta x^2\rangle &= \frac{1}{\gamma^2}\left\langle \left(\int_0^\infty \mathrm{d}\tau_1\, f(t-\tau_1)\chi(\tau_1)\right)\left(\int_0^\infty \mathrm{d}\tau_2\, f(t-\tau_2)\chi(\tau_2)\right)\right\rangle \\
&= \int_0^\infty \mathrm{d}\tau_1 \int_0^\infty \mathrm{d}\tau_2\, \langle f(t-\tau_1)f(t-\tau_2)\rangle \underbrace{\chi(\tau_1)\chi(\tau_2)}_{=\frac{1}{\gamma^2}\exp\left(-\frac{\tau_1+\tau_2}{\sigma}\right)} \\
&= \int_0^\infty \mathrm{d}\tau_1 \int_{-\tau_1}^\infty \mathrm{d}\tau\, \langle f(t-\tau_1)f(t-\tau_1-\tau)\rangle \frac{1}{\gamma^2}\exp\left(-\frac{2\tau_1+\tau}{\sigma}\right) \\
&= \int_0^\infty \mathrm{d}\tau_1 \int_{-\infty}^\infty \mathrm{d}\tau\, \langle f(t-\tau_1)f(t-\tau_1-\tau)\rangle \frac{1}{\gamma^2}\exp\left(-\frac{2\tau_1+\tau}{\sigma}\right) + \mathcal{O}(D\tau_m) \\
&= \frac{1}{\gamma^2}\int_0^\infty \mathrm{d}\tau_1 \exp\left(-\frac{2\tau_1}{\sigma}\right)\int_{-\infty}^\infty \mathrm{d}\tau\, \langle f(t-\tau_1)f(t-\tau_1-\tau)\rangle \underbrace{\exp\left(-\frac{\tau}{\sigma}\right)}_{\approx 1,\, \tau_m \ll \sigma} \\
&= \frac{1}{\gamma^2}\frac{\sigma}{2}2D\gamma^2 = \frac{\gamma}{k}D
\end{aligned}$$

At this point, we would like to make use of the equipartition theorem

$$\left\langle \frac{k}{2}x^2 \right\rangle = \frac{k_B T}{2} \tag{2.24}$$

As we have

$$\left\langle \frac{k}{2}x^2 \right\rangle = \frac{k}{2}\frac{\gamma}{k}D = \frac{k_B T}{2} \tag{2.25}$$

we obtain the Stokes-Einstein-relation

$$D = \frac{k_B T}{\gamma} \tag{2.26}$$

Numerical Solution: Explicit Euler Scheme

Consider as a heuristic example a stochastic process where inertia is negligible

$$\gamma \dot{x} = f(t) \tag{2.27}$$

A numerical solution for e.g. a particles position $x(t)$ depending on the random force $f(t)$ can be obtained from an explicit Euler scheme for discrete times $t_n = n \cdot dt$ and discrete positions $x_n = x(t_n)$.

The updates

$$u_n = \int_{t_n}^{t_{n+1}} dt \frac{f(t)}{\gamma} \tag{2.28}$$

have the properties

$$\langle u_n \rangle = 0, \quad \langle u_n^2 \rangle = 2Ddt, \quad \langle u_n u_{n+1} \rangle \approx 0 \tag{2.29}$$

The can be parameterized via $u_n \approx \sqrt{2D}dw_n$, where $dw_n \sim N(0, dt)$ are independent, normally distributed random variables. Finally, the explicit Euler scheme reads

$$x_{n+1} = x_n + \sqrt{2D}dw_n \tag{2.30}$$

One needs to be careful if $D = D(x)$.

Examples for Diffusion Processes

The damping of a colloid with radius r constant is given by $\gamma = 6\pi\eta r$.

For $r = 1\,\mu\text{m}$ and the viscosity of water $\eta = 1 \cdot 10^{-3}\,\text{Pa s}$ this yields $\gamma = 2 \cdot 10^{-8}\,\text{N s m}^{-1}$ and $D = \frac{k_B T}{\gamma} = 2 \cdot 10^{-13}\,\text{m}^2\,\text{s}^{-1}$

For a protein with $r = 2\,\text{nm}$ in water this yields $\gamma = 4 \cdot 10^{-11}\,\text{N s m}^{-1}$ and $D = \frac{k_B T}{\gamma} = 1 \cdot 10^{-10}\,\text{m}^2\,\text{s}^{-1}$

3 Langevin Equation and Fokker-Planck Equation

3.1 Langevin equation

Langevin equations are prototypical stochastic differential equations, which describe a wide variety of stochastic processes with many applications in different fields of physics (and beyond). Usually, Langevin equations comprise a deterministic part that describes the dynamics in the absence of noise, plus a stochastic noise term given by Gaussian white noise. An example would be Brownian motion of a suspended particle as discussed above, if the (physical) fluctuating force term is idealized as Gaussian white noise. The Fokker-Planck equation is a partial differential equation for the time evolution of the probability density of a stochastic processes given by a Langevin equation.

Definition of the Langevin equation

A *Langevin equation* is a stochastic differential equation for a stochastic process $x(t)$ (e.g., the x-position of a diffusing particle)

$$\dot{x} = \underbrace{f(x)}_{\text{drift}} + \underbrace{\sqrt{2D}\,\xi(t)}_{\text{random noise}} \tag{3.1}$$

- $f(x)$ is a deterministic drift term
- $\xi(t)$ represents Gaussian white noise with $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$

We can interpret $x(t)$ as the overdamped dynamics of a particle with position $x(t)$ in an effective potential $U(x) = -\int_0^x \mathrm{d}x'\, f(x')$ subject to noise. (This effective potential still has physical units of an acceleration, and would have to be multiplied by the friction coefficient γ of the particle to obtain the proper physical unit of a potential.)

Generalisation to n variables

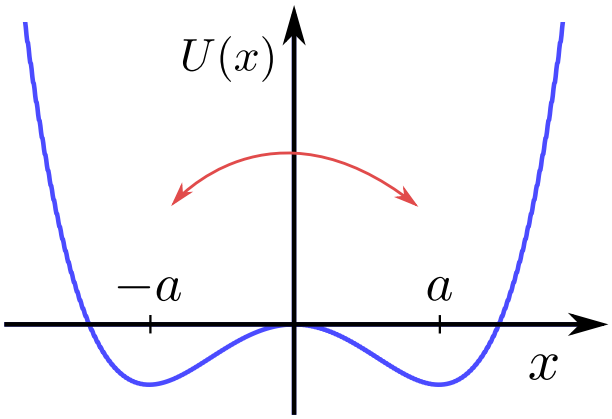
In an analogous way, we define Langevin equation for n variables

$$\dot{x}_i = f_i(\vec{x}, t) + \sum_{j=1}^{m} g_{ij}(\vec{x})\xi_j(t) \quad ,$$

i = 1, . . . , n , (3.2)where $\xi_j(t)$ are independent Gaussian white noise terms with $\langle \xi_j(t)\xi_l(t')\rangle = \delta_{jl}\delta(t-t')$, $j, l = 1, \ldots, m$.

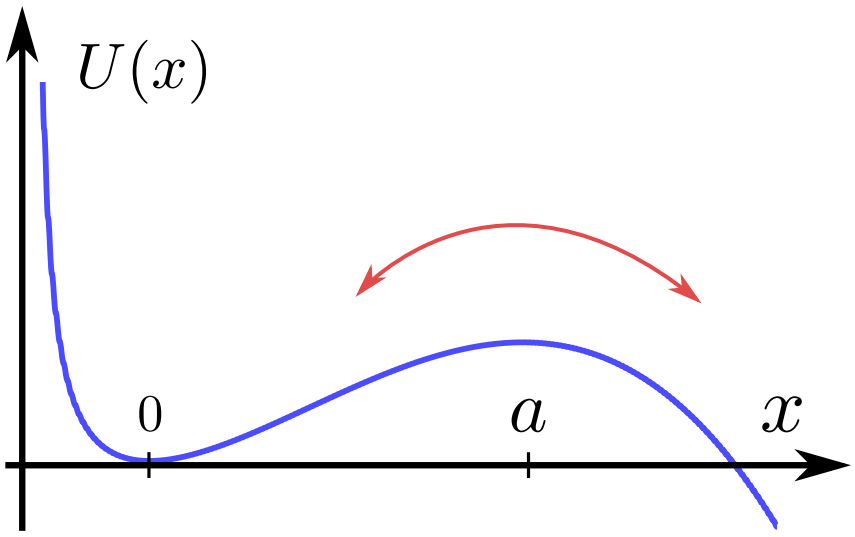
We announce three examples that will be treated in detail later in the lecture.

Example I: Double-well Potential



Assume, $x(t)$ obeys the Langevin equation $\dot{x} = -dU/dx + \xi(t)$, where $U(x)$ is a double-well potential as shown in the sketch. Noise will cause stochastic transitions between the left and right well. More generally, we can consider an ensemble of realizations $x(t)$. with the same initial condition $x(t = 0) = a$. For the time-dependent probability density $p(x, t)$ of this ensemble, we thus have $p(x, t = 0) = \delta(x - a)$. As time proceeds, this initial δ-peak will broaden, until this peak has equilibrated in the right well. At the same time, some realizations will transition to the left well. At the steady-state, this current from the right to the left well is exactly balanced by a current going in the opposite direction. We will show below that the steady-state distribution is given by a Boltzmann distribution $p^*(x) = \lim_{t\to\infty} p(x, t) \sim \exp(-U(x)/D)$.

Example II: Escape over a Barrier



Similarly, we can consider a potential $U(x)$ that drops to $-\infty$ for $x \gg a$, with this drop separated from a potential minimum at $x = 0$ by a potential barrier of height ΔU, as shown in the sketch. Noise can drive a particle starting at $x(t = 0) = 0$ over the barrier. For an ensemble of particles, this defines an (asymptotic) *escape rate*, at which particles still in the well escape over the barrier. (The backward current over the barrier back to $x \approx 0$ is negligible.) Later, we will compute this escape rate as function of ΔU using Kramer's escape rate theory.

Example III: Synchronization

As an example of coupled Langevin equations, we consider the synchronization of $n = 2$ noisy oscillators with respective oscillator phases $\varphi_1(t)$ and $\varphi_2(t)$, whose stochastic dynamics is given by

$$\dot{\varphi}_1 = \omega_0 + \lambda \sin(\varphi_1 - \varphi_2) + \xi_1(t) \tag{3.3}$$

$$\dot{\varphi}_2 = \omega_0 - \lambda \sin(\varphi_1 - \varphi_2) + \xi_2(t) \quad , \tag{3.4}$$

with identical angular frequency ω_0, a sinusoidal coupling term with coupling strength λ, and independent Gaussian white noise terms $\xi_1(t)$ and $\xi_2(t)$ with $\langle \xi_i(t)\xi_j(t)\rangle = 2D\,\delta_{ij}, \delta(t-t')$, $i, j = 1, 2$. In the absence of noise with $D = 0$, the two oscillators will synchronize in-phase with phase difference $\delta(t) = \varphi_1(t) - \varphi_2(t) = 0$ provided $\lambda > 0$. In the presence of noise with $D > 0$, the phase difference $\delta(t)$ will fluctuate around a value $2\pi\, k$ for integer k with occasional, noise-induced *phase slips* during which $\delta(t)$ increases in relatively short time by $\pm 2\pi$.

Numerics for the Langevin Equation

We can numerically integrate Langevin equations using the Euler-Maruyama scheme, which generalizes the well-known Euler scheme to the case of stochastic differential equations.

Euler-Maruyama Scheme

Let $t_j = j\ \mathrm{d}t$ be equidistant time points separated by a small time step $\mathrm{d}t$. We seek to estimate the value $\hat{x}_{j+1} \equiv x(t_j)$ of a stochastic realization of the Langevin equation $\dot{x} = f(x) + \sqrt{2D}\,\xi(t)$, where $\xi(t)$ denotes Gaussian white noise with $\langle \xi(t)\xi(t')\rangle = \delta(t-t')$. The Euler-Maruyama scheme specifies the following update-rule

$$\hat{x}_{j+1} = \hat{x}_j + f(\hat{x}_j)\,\mathrm{d}t + \sqrt{2D\,\mathrm{d}t}\Delta W_j \tag{3.5}$$

with independent normal distributed random numbers $\Delta W_j \sim N(0,1)$ with mean zero and variance one.

Remark: For finite time step $\mathrm{d}t$, a numerical error on the order $\mathcal{O}(\mathrm{d}t^{3/2})$ occurs. In the limit $\mathrm{d}t \to 0$, we may interpret solutions of this Euler-Maruyama scheme as a definition of a stochastic realization of the Langevin equation $\dot{x} = f(x) + \sqrt{2D}\,\xi(t)$.

Remark: For the numerical integration of ordinary differential equations, higher-order schemes (such as Runge-Kutta schemes) are often useful. In contrast, for the numerical integration of stochastic differential equations, the added complexity of higher-order schemes makes these less useful and the simple Euler-Maruyama scheme is often a good choice for practical applications. Intuitively, higher-order schemes allow to reduce numerical errors, but for stochastic differential equations, numerical errors are "masked" by the noise term anyway.

Caution: Care needs to be taken in cases where the noise strength depends on the current state, i.e., $D = D(x)$, because different update schemes give different results in this case, corresponding to different "interpretations" of the Langevin equation, see later chapter on Ito and Stratonovich calculus.

3.2 Fokker-Planck-Equation

We are interested in the time evolution of an *ensemble* of realizations $x(t)$ of a Langevin equation, which is characterized by a time-dependent *probability density* $p(x,t)$. We will derive a partial differential equation that describes the time-evolution of $p(x,t)$, the famous Fokker-Planck equation.

Example: Diffusion equation The diffusion equation of a freely diffusing particle already

is an example of a Fokker-Planck equation. We consider a particle diffusing in one space dimension with position $x(t)$, described by the Langevin equation

$$\dot{x} = \xi(t) \quad , \tag{3.6}$$

where $\xi(t)$ is Gaussian white noise with $\langle \xi(t)\xi(t') \rangle = 2D\,\delta(t-t')$. For the initial condition $x(0) = 0$, the probability density is given by normal distribution with time-dependent variance

$$p(x,t) = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{2Dt}} \exp\left(-\frac{x^2}{4Dt}\right) \quad . \tag{3.7}$$

Note $\langle x(t) \rangle = 0$ and $\langle x^2(t) \rangle = 2D\,t$. This probability density satisfies the *diffusion equation*

$$\frac{\partial p(x,t)}{\partial t} = D \frac{\partial^2 p(x,t)}{\partial x^2} \quad . \tag{3.8}$$

In fact, we could have started with any initial probability distribution $p(x, t = 0)$ and the time evolution will still be given by the diffusion equation.

Derivation of Fokker-Planck-Equation

Considering the general case $\dot{x} = f(x) + \sqrt{2D}\,\xi(t)$, we would like to find an operator $\hat{L}$ such that

$$\frac{\partial p(x,t)}{\partial t} = \hat{L} p(x,t) \tag{3.9}$$

Therefore, we discretize time and take a look how a sub-ensemble of $p(x,t)$ at x_n will evolve during a time step from $p(x,t_n)$ to $p(x,t_{n+1})$. For this we are using the Markov-Property:

$$\begin{aligned} p(x,t_{n+1}|x_0,t_0) &= \int \mathrm{d}x_n\, p(x,t_{n+1},x_n,t_n|x_0,t_0) \\ &= \int \mathrm{d}x_n\, p(x,t_{n+1}|x_n,t_n)\, p(x_n,t_n|x_0,t_0) \\ &= \int \mathrm{d}x_n\, N(x_n + f(x_n), 2D\,\mathrm{d}t) p(x_n,t_n|x_0,t_0) \end{aligned}$$

The left term captures the probability to have been at x_n at $t = t_n$, the right term the probability to have moved from x_n to x_{n+1}.

This is already an implicit solution in terms of a convolution of the probability density with a family of normal distributions, but it is of little practical use.

A Remark about Units

Unlike probabilities, probability densities for positions have units of inverse length! Therefore we are integrating over a two-point probability density which has units of inverse length squared

$$[p(x, t_{n+1}|x_0, t_0)] = \mathrm{m}^{-1}$$
$$[p(x, t_{n+1}, x_n, t_n|x_0, t_0)] = \mathrm{m}^{-2}$$

So, let us define the following abbreviations in order to evaluate this convolution further

$$p(x, t_n) = \int \mathrm{d}x_n I(x_n, y)|_{y=x-x_n} \quad \text{with} \quad I(x_n, y) = p(x_n)n(x_n, y),$$
$$\text{and} \quad n(x_n, y) = N(f(x_n)\mathrm{d}t, 2D\mathrm{d}t)$$

The integrand $I(x, y)$ will contribute only for small $y = \mathcal{O}(\mathrm{d}t)$, which means $x_n \approx x$, so we can Taylor expand $I(x_n, y)$ in x_n around x:

$$I(x_n, y) = I(x, y) + \frac{\partial I(x_n, y)}{\partial x_n}\Big|_{x_n=x}(x_n - x) + \frac{\partial^2 I(x_n, y)}{\partial x_n^2}\Big|_{x_n=x}\frac{(x_n - x)^2}{2} \tag{3.10}$$

Inserting this into the convolution integral leads to

$$\begin{aligned} p(x, t_{n+1}) &= \int \mathrm{d}y\, I(x, y)|_{x_n=x-y} \\ &= \int \mathrm{d}y \left(p(x)n(x, y) - \frac{\partial}{\partial x}(p(x)\, n(x, y)\, y) + \frac{\partial^2}{\partial x^2}\left(p(x)\, n(x, y)\, \frac{y^2}{2}\right)\right) \\ &= p(x) \int \mathrm{d}y\, n(x, y) - \frac{\partial}{\partial x}\left(p(x) \int \mathrm{d}y\, n(x, y)\, y\right) + \frac{\partial^2}{\partial x^2}\left(p(x) \int \mathrm{d}y\, n(x, y)\, \frac{y^2}{2}\right) \end{aligned}$$

The integrals that are occurring in this step are know as Kramers-Moyal coefficients:

$$\int \mathrm{d}y\, n(x,y) = 1$$
$$\int \mathrm{d}y\, n(x,y)\, y = f(x)\,\mathrm{d}t$$
$$\int \mathrm{d}y\, n(x,y)\, \frac{y^2}{2} = D\,\mathrm{d}t + \frac{1}{2}[f(x)]^2\,\mathrm{d}t^2 = D\,\mathrm{d}t + \mathcal{O}(\mathrm{d}t^2)$$

which give us

$$p(x,t_{n+1}) = p(x,t_n) - \frac{\partial}{\partial x}[p(x,t_n)f(x)\,\mathrm{d}t] + \frac{\partial^2}{\partial x^2}[p(x,t_n)D]\,\mathrm{d}t \tag{3.11}$$

and thus

$$\frac{p(x,t_{n+1}) - p(x,t_n)}{\mathrm{d}t} = -\frac{\partial}{\partial x}[p(x,t_n)f(x)] + \frac{\partial^2}{\partial x^2}[p(x,t_n)D] \tag{3.12}$$

Taking the time step to zero, we have finally derived the Fokker-Planck equation.

Fokker-Planck equation

The Fokker-Planck equation is a partial differential equation for a probability density $p(x)$, which reads for an ensemble governed by the Langevin equation (3.1) as follows

$$\frac{\partial}{\partial t}p(x,t) = -\frac{\partial}{\partial x}[p(x,t)\,f] + D\frac{\partial^2}{\partial x^2}p(x,t) \tag{3.13}$$

The structure of the Fokker-Planck equation is similar to the Schrödinger equation, i.e. solution methods from QM can be borrowed (take a look at the Risken book [**Risken1996**]).

Application to Diffusion in a Potential

We consider diffusion in a potential $U(x)$ (now we care about physical units!)

$$\dot{x} = -\frac{1}{\gamma}\frac{\partial U}{\partial x} + \xi \tag{3.14}$$

and ask for the steady state $\frac{\partial}{\partial t}p(x,t) = 0$. Hence, the Fokker-Planck equation reads

$$\begin{aligned} 0 &= \vec{\nabla}[(\frac{1}{\gamma}\vec{\nabla}U)p] + D\vec{\nabla}^2 p = \vec{\nabla}[\frac{1}{\gamma}\vec{\nabla}Up + D\vec{\nabla}p] \\ \Rightarrow c &= \frac{1}{\gamma}\vec{\nabla}Up + D\vec{\nabla}p \end{aligned}$$

thus, if $c = 0$, we get

$$\frac{\partial}{\partial x}\ln p = \frac{\vec{\nabla}p}{p} = -\frac{1}{\gamma}\frac{\vec{\nabla}U}{p} \tag{3.15}$$

and

$$p \sim \exp\left(-\frac{U}{\gamma D}\right) = \exp\left(-\frac{U}{k_B T}\right) \tag{3.16}$$

with $D = \frac{k_B T}{\gamma}$, i.e. we recover the Boltzmann distribution. If c would not be zero, the solution could not be normalized. Another explanation, why $c = 0$, is based on the Fokker-Planck-equation being interpreted as conservation equation

$$\dot{p} = -\vec{\nabla}\vec{J} \quad \text{with} \quad \vec{J} = \frac{1}{\gamma}\vec{\nabla}Up + D\vec{\nabla}p \tag{3.17}$$

of the current $\vec{J}$. At equilibrium, the current must vanish and thus we have

$$\lim_{t\to\infty}\vec{J} = c = 0 \tag{3.18}$$

Eigenvalue Spectrum of $\hat{L}$

The probability density can be expressed in terms of eigenfunctions of the Fokker-Planck operator $\hat{L}$ with $\dot{p} = \hat{L}p$

$$\hat{L}\phi_n(x) = \lambda_n\phi_n(x) \tag{3.19}$$

through

$$p(x,t) = \sum a_n\phi_n(x)\exp(\lambda_n t) \tag{3.20}$$

If $\lambda_0 = 0$, then the corresponding eigenfunction is a steady state ϕ_0. The slowest decaying mode determines hopping rates and it is $0 \leq \lambda_1 \leq \lambda_2 \ldots$.

But why are the λ_n real? We have $\hat{L} \neq \hat{L}^*$, which means $\hat{L}$ is not Hermitian.

$$\left\langle \hat{L}g, h \right\rangle = \int \mathrm{d}x\, (\hat{L}g)h = \int \mathrm{d}x\, g\hat{L}^* h = \left\langle g, \hat{L}^* h \right\rangle \quad \forall g(x), h(x) \tag{3.21}$$

By partial integration we see that the adjoint operator has the form

$$\hat{L}^* h = f\frac{\partial h}{\partial x} + D\frac{\partial^2 h}{\partial x^2} \tag{3.22}$$

If $f(x) = -\frac{\partial U(x)}{\partial x}$, we can define a Hermitian operator by

$$A = T^{-1}LT \quad \text{with} \quad T = \exp\left(+\frac{\beta U}{2}\right),\ \beta = \frac{1}{D} \tag{3.23}$$

The operator is self-adjoint $\hat{A} = \hat{A}^*$ and thus all eigenvalues are real. $\hat{A}$ and $\hat{L}$ have the same eigenvalues.

Backward Fokker-Planck Equation

$p = p(x_1, t|x_0, 0) = p(x_1, 0|x_0, -t)$, which gives the backward Fokker-Planck equation

$$\dot{p} = \hat{L}_{x_1} p = \hat{L}^*_{x_0} p = \left[+f(x)\frac{\partial}{\partial x_0} + D\frac{\partial^2}{\partial x_0^2}\right] p(x_1, 0\,|\,x_0, -t) \tag{3.24}$$

Boundary Conditions Matter

1) Reflecting Boundary Conditions (No-Flux / Robin B.C.)

The probability current $\dot{p} = -J$ vanishes

$$J(x_1) = J(x_2) = 0 \tag{3.25}$$

and

$$\int_{x_1}^{x_2} \mathrm{d}x\, p(x,t) = 1 \to \frac{\mathrm{d}}{\mathrm{d}t}\int_{x_1}^{x_2} \mathrm{d}x\, p(x,t) = 0 \tag{3.26}$$

In this case the steady-state distribution $p^*(x) = \phi_0(x)$ exists. Similar results hold for a confinement potential $\lim_{x\to x_1,x_2} U(x) \to \infty$.

2) Absorbing Boundary Conditions

For absorbing boundary conditions we impose $p(x_2, t) = 0$ (Dirichlet boundary conditions). Therefore

$$0 > \frac{\mathrm{d}}{\mathrm{d}t}\int \mathrm{d}x\, p(x,t) = \int \mathrm{d}x\, \frac{\mathrm{d}p(x,t)}{\mathrm{d}t} = \int_{-\infty}^{x_2} -\frac{\partial J}{\partial x} = -J(x_2) \tag{3.27}$$

is the flux to the absorber.

No steady-state solution exists (non-trivial / normalizable to one) and all eigenvalues are strictly negative. $\lambda_1 < 0$ sets the slowest time scale.

In the limit of long times $t \to \frac{1}{\lambda_1}$, the porbability density can be decomposed into $p(x,t) = a(t)p_1(x)$ with $a(t) \sim \exp(-\lambda_1 t)$.

Boundary Conditions and Functional Analysis

Changing the boundary conditions changes also the eigenvalues and the adjoint operator (boundary terms might pop up) and thus you will get each time a different operator in terms of functional analysis.

3.3 Master Equation

The master equation (M-equation) describes time-continuous, continuous state variables and it is of the general form

$$\frac{\partial}{\partial t}P(x,t) = \int \mathrm{d}x_1 \underbrace{w(x|x_1)P(x_1,t)}_{=\text{gain}} - \underbrace{w(x_1|x)P(x,t)}_{=\text{loss}} \tag{3.28}$$

$w(x|x_1)$ is the transition rate density for the process $x_1 \to x_2$, i.e. $w(x|x_1)\Delta x_1 \Delta x_2 \Delta t$ is the probability of a transition from $[x_1, x_1 + \Delta x_1]$ to $[x_2, x_2 + \Delta x_2]$ in the time interval Δt

The Fokker-Planck equation is a special case of the master equation.

For a time-continuous, discrete state variable the master equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}P_n(t) = \sum_m w_{nm}p_m(t) - w_{mn}p_n(t) \tag{3.29}$$

where w_{nm} is the transition rate $m \to n$.

Example I: Fermi's Golden Rule

Let $\hat{H} = \hat{H}_0 + \varepsilon\hat{H}_1\Theta(t)$ be a perturbed Hamiltonian and $|m_0\langle$ be an eigenstate of the unperturbed Hamiltonian $\hat{H}_0$ and the initial state.

The transition rate $m_0 \to n$ is given by Fermi's Golden rule

$$w_{nm_0} = \frac{2\pi}{\hbar}\varepsilon^2|\langle n|\hat{H}_1|\rangle|\rho + \mathbb{O}(\varepsilon^4) \tag{3.30}$$

Example II: Radioactive Decay

Let n be the number of particles that is left (i.e. not decayed).

$$T_{\delta t}(n|m) = \begin{cases} 0 & n > m \\ m\gamma\delta t & n = m \\ \mathbb{O}(\delta t^2) & n < m \end{cases} \tag{3.31}$$

The master equation reads

$$\frac{\mathrm{d}}{\mathrm{d}t}p_n = \gamma(n+1)p_{n+1} - \gamma(n)p_n \tag{3.32}$$

where $N = \langle n\rangle = \sum_n p_n$ and

$$\frac{\mathrm{d}}{\mathrm{d}t}N = -\gamma(n)N \tag{3.33}$$

and thus $N = N_0\exp(-\gamma t)$.

4 Dynkin Equation

4.1 Mean First Passage Times and Dynkin Equation

We consider diffusion in some potential landscape $\gamma\dot{x} = -\frac{\partial U}{\partial x} + \xi(t)$ with initial conditions $p(x,0) = \delta(x - x_1)$ and absorbing boundary conditions $p(x_2,t) = 0$, i.e, $\dot{p} = -\nabla J$ where $J(x_2,t)$ is the current to the absorbing boundary conditions.

> **Mean First Passage Time (MFPT)**
>
> $$\tau(x_2|x_1) = \int_0^\infty \mathrm{d}t\, t J(x_2,t|x_1,0) \tag{4.1}$$

Our goal is to derive an equation for τ in the process

$$x_1 \underbrace{\longrightarrow}_{\Delta t} x' \underbrace{\longrightarrow}_{\tau(x_2|x')} x_2 \tag{4.2}$$

If Δt is small and kept constant (and we ask which positions can we reach within Δt) we have

$$\tau(x_2|x_1) = \Delta t + \int_{-\infty}^{x_2} \mathrm{d}x'\, \tau(x_2|x') p(x',\Delta t|x_1,0) \tag{4.3}$$

and we take the derivative with respect to Δt

$$\frac{\mathrm{d}\tau(x_2|x_1)}{\mathrm{d}\Delta \mathrm{t}} = 0 = 1 + \int_{-\infty}^{x_2} \mathrm{d}x'\, \tau(x_2|x') \hat{L}_{x'} p = 1 + \int_{-\infty}^{x_2} \mathrm{d}x'\, \hat{L}^*_{x'} \tau(x_2|x') p \tag{4.4}$$

so, if $\Delta t \to 0$ then $p(x',\Delta t|x_1,0) \to \delta(x - x_1)$, and we get the *Dynkin equation*

$$-1 = \hat{L}^*_{x_1} \tau(x_2|x_1) \tag{4.5}$$

Application to Diffusion

Let consider once again the example of diffusion

$$\gamma\dot{x} = -\frac{\partial U}{\partial x} + \xi(t) \quad \langle \xi(t)\xi(t')\rangle = 2D\delta(t-t') \tag{4.6}$$

with the initial condition $p(x,0) = \delta(x - x_1)$ and boundary conditions $p(x_2, t) = 0$. Let $v = \frac{\partial}{\partial x_1}\tau(x_2|x_1)$, so the Dynkin equation reads

$$-1 = Dv' - \frac{U'}{\gamma}v \tag{4.7}$$

which we multiply by $\frac{1}{D}\exp(-\beta U)$

$$-\frac{1}{D}\exp(-\beta U) = v'\exp(-\beta U) - \beta v\exp(-\beta U) = \frac{\mathrm{d}}{\mathrm{d}x_1}[v\exp(-\beta U)] \tag{4.8}$$

to get

$$v = -\frac{1}{D}\exp(-\beta U)\left[\int_{-\infty}^{x_1}\mathrm{d}x'\exp(-\beta U) + c\right] \tag{4.9}$$

If we assume $\lim_{x\to-\infty} U(x) = +\infty$, then $|v| < \infty$ and $c = 0$. With one more integration we get

$$\tau(x_2, x_1) = \frac{1}{D}\int_{x_1}^{x_2}\exp(\beta U(x'))\left[\int_{-\infty}^{x'}\mathrm{d}x''\exp(-\beta U(x''))\right] \tag{4.10}$$

Note that the integration constant of the second integration must be zero due to $\tau(x_2|x_2) = 0$

4.2 Kramers Escape Rate Theory

We consider the escape of particles over an energy barrier ΔE and assume $\beta\Delta E \gg 1$ to calculate $\tau(x_2|x_1)$. $\int \mathrm{d}x''$ is sizeable only nearby x_a, $\int \mathrm{d}x'$ is sizeable only nearby x_b. We

do a standard trick: quadratic expansion around x_a and x_b

$$U(x'') = U(x_a) + \frac{1}{2}U''(x_a)(x'' - x_a)^2 + \dots \tag{4.11}$$

with $U''(x_a) = k_a = \gamma/\tau_a$, which introduces a time-scale. Similarly

$$U(x') = U(x_b) + \frac{1}{2}U''(x_b)(x' - x_b)^2 + \dots \tag{4.12}$$

with $U''(x_b) = -k_b = -\gamma/\tau_b$. So lets evaluate our integrals

$$\begin{aligned}\int_{-\infty}^{x'} \mathrm{d}x'' \exp\left(-\frac{1}{2}\beta U''(x_a)(x'' - x_a)^2\right) &\approx \int_{-\infty}^{\infty} \mathrm{d}x'' \exp\left(-\frac{1}{2}\beta U''(x_a)(x' - x_a)^2\right) \\ &= \sqrt{2\pi\sigma^2}\end{aligned}$$

with $\sigma^2 = \frac{\tau_a}{\beta\gamma}$ and

$$\begin{aligned}\int_{-\infty}^{x'} \mathrm{d}x'' \exp\left(+\frac{1}{2}\beta U''(x_b)(x' - x_b)^2\right) &\approx \int_{-\infty}^{\infty} \mathrm{d}x'' \exp\left(+\frac{1}{2}\beta U''(x_b)(x' - x_b)^2\right) \\ &= \sqrt{2\pi\frac{\tau_b}{\beta\gamma}}\end{aligned}$$

so

$$\tau(x_2|x_1) = \frac{1}{D}\frac{2\pi\sqrt{\tau_a\tau_b}}{\beta\gamma}\exp(\beta\Delta E) = 2\pi\sqrt{\tau_a\tau_b}\exp(\beta\Delta E) \tag{4.13}$$

Kramers escape rate

$$r = \frac{1}{\tau(x_2|x_1)} \sim \underbrace{\exp(-\beta\Delta E)}_{\text{Arrheniusfactor}} \tag{4.14}$$

4.3 Diffusion to Capture

As an example, we consider a diffusing particle released at position x_0 between two absorbing plates at positions x_1 and x_2.

The question is: What is the probability of getting absorbed at either of the two plates?

$$P(x, t = 0) = \delta(x - x_0)$$
$$P(x_1, t) = P(x_2, t) = 0$$

The probability of becoming absorbed at $x = x_1$ when starting at x_0 reads $\pi_1(x_0)$. We have $\pi_1(x_1) = 1$ and $\pi_1(x_2) = 0$.

Solution 1

We will now consider a time step Δt as we did for the derivation of the Dynkin equation in order to find an explicit expression for $\pi_1(x_0)$:

$$\pi_1(x_0) = \int_{x_1}^{x_2} \mathrm{d}x\, \pi_1(x) P(x, \Delta t | x_0, 0) = \int_0^\infty \mathrm{d}t\, J(x_1, t | x_0, 0)$$

Now we take the partial derivative with respect to Δt

$$0 = \int_{x_1}^{x_2} \mathrm{d}x\, \pi_1(x) \underbrace{\frac{\partial}{\partial \Delta t} P(x, \Delta t | x_0, 0)}_{\hat{L}P}$$

and perform partial integration

$$0 = \int_{x_1}^{x_2} \mathrm{d}x\, \hat{L}^* \pi_1(x)\, \underbrace{P(x, \Delta t | x_0, 0)}_{\to \delta(x - x_0) \text{ for } \Delta t \to 0}$$

so we obtain

$$0 = \hat{L}^* \pi_1(x)$$

Thus, $\pi_1(x_0)$ must be a linear function and taking the boundary conditions into account we conclude $\pi_1(x_0) = \frac{x_2 - x_0}{x_2 - x_1}$.

Solution 2

Another way to compute this is the method of images. So

$$P(x,t) = N(x_0, 2Dt) - N(2x_1 - x_0, 2Dt) - N(2x_2 - x_0, 2Dt) \tag{4.15}$$

and π_1 could be calculated directly. (Stream of anti-particles is released and annihilates particles at the boundary).

4.4 Polya's theorem

We consider diffusion in $\mathbb{R}^d$ to a d-dimensional absorbing ball. We ask for the probability $p(R_0)$ for a particle initially released at distance R_0 to hit the target ball. For $d = 1$ and $d = 2$ we have $p(R_0) = 1$, but for $d = 3$ $p(R_0) = \frac{R_1}{R_0}$

Note that for $d = 3$, the characteristic arrival time must scale with $\sqrt{R_0^2/D}$ with a power-law tail $\sim t^{-3/2} \exp(-(R_0 - R_1)^2/4Dt)$ and the mean first passage time diverges.

5 Active Oscillators and Synchronization

This chapter will introduce different examples for so-called *active oscillators*, i.e. non-conservative oscillators loosing energy through damping, such as

- Van-der-Pol oscillator: $m\ddot{x} - \gamma\left(\frac{1}{4}\Lambda - x^2\right)\dot{x} + kx = 0$
- Hopf oscillator: $\dot{z} = i\omega_0 z + \mu(\Lambda - |z|^2)z$
- Phase oscillator: $\dot{\varphi} = \omega_0$

We will also look at the intriguing phenomenon of synchronization between coupled oscillators.

5.1 Van-der-Pol Oscillator

This type of oscillator model was investigated first by Van-der-Pol when working at Phillips on electrical circuits with vacuum tube amplifiers [**Vanderpol1927**]. It was later adapted to model neurons (FitzHugh–Nagumo model) and in seismology to model geological faults.

Van-der-Pol Oscillator

$$m\ddot{x} - \gamma\left(\frac{1}{4}\Lambda - x^2\right)\dot{x} + kx = 0 \tag{5.1}$$

The Van-der-Pol oscillator undergoes a so-called Hopf bifurcation as a function of parameter Λ: For $\Lambda < 0$ $x = 0$ it is stable and for $\Lambda > 0$ limit-cycle oscillations occur. Equation (5.1) can be transformed into Hopf normal form.

Hopf normal form of Van-der-Pol oscillator

We set $y = \dot{x}$, $\omega = \sqrt{k/m}$. The idea is to introduce $z \approx x - \frac{i}{\omega}y$, so we do the ansatz (in order to avoid quartic terms / the method is called Center Manifold technique)

$$\begin{aligned} z &= \sum_k^\infty \sum_l^\infty d_{k,l} x^l y^{k-l} \\ &= x - \frac{i}{\omega}y + d_{10}y + d_{33}x^3 + d_32x^2y + d_{31}xy^2 + d_{30}y^3 + \dots \end{aligned}$$

The back transformation is given by

$$\begin{aligned} x &= \frac{z+\bar{z}}{2} + e_1 z^3 + e_2 z^2\bar{z} + e_3 z\bar{z}^2 + e_4\bar{z}^3 \dots \\ y &= i\omega\frac{z-\bar{z}}{2} + f_1 z^3 + f_2 z^2\bar{z} \dots \end{aligned}$$

so that

$$\dot{z} = h(z,\bar{z}) = Fz + Gz^2\bar{z} + \text{h.o.t.} \tag{5.2}$$

and for appropriate $d_{k,l}$ we have i) no quadratic terms, ii) no term in $\bar{z}$ and iii) no terms proportional to $z^3, z\bar{z}^2, \bar{z}^3$. We find that

$$\begin{aligned} F &= i\omega_0 + \frac{\gamma}{8m}\Lambda + \mathcal{O}(\Lambda^2) \\ G &= \frac{\gamma}{8m} + \mathcal{O}(\Lambda) \end{aligned}$$

and we get

$$\dot{z} = i(\omega_c - \omega_1|z|^2)z + \mu(\Lambda - |z|^2) \tag{5.3}$$

with $\omega_c = \omega_0$, $\omega_1 = \mathcal{O}(\Lambda)$ and $\mu = \frac{\gamma}{8m}$

5.2 Hopf-Oscillator with Noise

Hopf oscillator

An active oscillator with non-linear damping of the form

$$\dot{z} = i\omega_0 z + \mu(\Lambda - |z|^2)z \quad \text{with} \quad z \in \mathbb{C} \tag{5.4}$$

It is used e.g. to describe the limit cycle of electric circuits involving a vacuum tube or in biology to model the activation potential of neurons.

We now add a noise term to the Hopf-oscillator

$$\dot{z} = i\omega_0 z + \mu(\Lambda - |z|^2)z + (i\xi_\varphi + \xi_A)z \tag{5.5}$$

with

$$\langle \xi_\varphi(t)\xi_\varphi(t')\rangle = 2D_\varphi\delta(t-t') \quad \langle \xi_A(t)\xi_A(t')\rangle = 2D_A\delta(t-t') \quad \langle \xi_\varphi(t)\xi_A(t')\rangle = 0$$

We map z on a phase φ and amplitude A via $z = Ae^{i\varphi}$ so that

$$\left(\frac{\dot{A}}{A} + i\dot{\varphi}\right) z = \dot{z} = \dots \tag{5.6}$$

and

$$\frac{\dot{A}}{A} + i\dot{\varphi} = i\omega_0 + \mu(A_0^2 - A^2) + i\xi_\varphi + \xi_A \tag{5.7}$$

Assuming $\Lambda > 0$ and $\Lambda = A_0^2$, we get a noisy phase oscillator

$$\dot{\varphi} = \omega_0 + \xi_\varphi \tag{5.8}$$

and an Ornstein-Uhlenbeck process for the amplitude

$$\begin{gathered} A = A_0 + a \\ \dot{a} = \mu(A_0 + a)(-2aA_0 + a^2) + \xi_A = -2\mu A_0 a + \xi_A + \mathcal{O}(a^2) \end{gathered} \tag{5.9}$$

with the properties

$$\langle a(t)\rangle = 0 \quad \langle a(t)a(t')\rangle = D_A\tau \exp\left\{-\frac{|t-t'|}{\tau}\right\} \quad \tau = \frac{1}{2\mu A_0}$$

Remark

If we consider an ensemble average, the amplitude fluctuations will decay with τ:

$$\bar{a}(t) = \langle a(t)\rangle \quad \text{with} \quad \frac{\mathrm{d}}{\mathrm{d}d}\bar{a} = -\frac{\bar{a}}{\tau}$$

Manifestation of Phase Noise

We can characterize noisy oscillations in terms of a phase correlation function

$$C(t) = \langle \exp(i\varphi(t_0)) \exp(-i\varphi(t_0+t))\rangle \tag{5.10}$$

with $|C(t) = \exp(-D_\varphi t)|$, so

$$\frac{z(t_0)}{A_0}\frac{\bar{z}}{A_0} \approx \exp(\varphi(t_0) - \varphi(t_0+t)) \to \exp(i\omega_0 t) \quad \text{if} \quad D_\varphi = 0$$

And we can have a look at the power spectral density

$$S_y(\omega) = |\tilde{y}(\omega)|^2 \tag{5.11}$$

with $y = \exp(i\varphi)$ and its Fourier transform $\tilde{y}(\omega)$.

5.3 Two coupled Phase Oscillators

Two phase oscillators are coupled by the coupling c leading to the ODE system

$$\begin{aligned} \dot{\varphi}_L &= \omega_L + c(\varphi_L - \varphi_R) \\ \dot{\varphi}_R &= \omega_R + c(\varphi_R - \varphi_L) \end{aligned} \tag{5.12}$$

We introduce a phase difference of $\delta = \varphi_L - \varphi_R$

$$\dot{\delta} = \Delta\omega + c(\delta) - c(-\delta) \tag{5.13}$$

with frequency mismatch $\Delta\omega = \omega_L - \omega_R$. A Fourier expansion of the coupling function yields

$$c(\delta) = c(\delta + 2\pi) = \sum_n C'_n \cos(n\delta) + C''_n \sin(n\delta) \tag{5.14}$$

Only the odd coupling terms contribute to synchronization, often $c(\delta)$ is dominated by the first Fourier mode and we end up at the Adler equation ($\lambda = -2c''_1$)

$$\dot{\delta} = \Delta\omega - \lambda \sin(\delta) \tag{5.15}$$

If $|\Delta\omega| < |\lambda|$, we have fixed points for $\delta^* = \sin^{-1}\left(\frac{\Delta\omega}{\lambda}\right)$. The stability of the fixed points is determined by $\gamma\dot{\delta} = -\frac{\partial U}{\partial \delta}$ and the effective potential $U = -\gamma\Delta\omega\delta - \gamma\lambda\cos(\delta)$.

Images missing!

5.4 Synchronization in the Presence of Noise

If we consider two coupled phase oscillators with noise

$$\dot{\varphi}_1 = \omega_1 - \frac{\lambda}{2}\sin(\varphi_1 - \varphi_2) + \xi_1(t) \tag{5.16}$$

$$\dot{\varphi}_2 = \omega_2 - \frac{\lambda}{2}\sin(\varphi_2 - \varphi_1) + \xi_2(t) \tag{5.17}$$

we obtain the noises Adler equation for the phase difference $\delta = \varphi_1 - \varphi_2$

$$\dot{\delta} = \Delta\omega - \lambda\sin(\delta) + \xi \tag{5.18}$$

Here, and Gaussian white noise $\xi(t)$ represents Gaussian white noise with $\langle \xi(t)\xi(t')\rangle = 2(D_L + D_R)\delta(t - t')$.

Remark: How to add two noise terms

$$\xi(t) = \xi_L(t) - \xi_R(t)$$

with $\langle \xi(t) \rangle = 0$ and

$$\begin{aligned}\langle \xi(t)\xi(t') \rangle &= \langle \xi_L(t)\xi_L(t') \rangle + \langle \xi_R(t)\xi_R(t') \rangle + \langle \xi_L(t)\xi_R(t') \rangle \\ &= 2D_L\delta(t-t') + 2D_R\delta(t-t') + 0 \\ &= 2(D_L + D_R)\delta(t-t')\end{aligned}$$

We can reinterpret the noisy Adler equation as the overdamped dynamics of a diffusing particle in a potential $U(x)$

$$\gamma\dot{\delta} = -\frac{\partial U}{\partial \delta} + \xi \tag{5.19}$$

and $U/\gamma = -\Delta\omega\delta - \lambda\cos(\delta)$. So what is the effect of noise? The steady state probability density reads

$$p^*(\delta) \sim \exp\left(-\frac{U(\delta)}{k_B T_{\text{eff}}}\right) = \frac{1}{2\pi I_0(ND)} \exp\left(-\frac{\lambda}{D}\cos(\delta)\right) \tag{5.20}$$

with $D = k_B T_{\text{eff}}\gamma$ and $\Delta\omega = 0$. So the first effect of noise is, that steady states are smeared out. The second effect are phase slips that occur

$$\begin{aligned}\delta \approx 0 \longrightarrow \delta \approx 2\pi \qquad &\text{with rate } G_+ \\ \delta \approx 0 \longrightarrow \delta \approx -2\pi \qquad &\text{with rate } G_-\end{aligned}$$

We can compute $G_\pm$ using Kramers escape rate theory

$$\frac{\gamma}{\tau_a} = U''|_{\delta=\delta_a} \Rightarrow \tau_a = \frac{1}{\sqrt{\lambda^2 - \Delta\omega^2}}$$

$$\frac{\gamma}{\tau_b} = U''|_{\delta=\delta_b} \Rightarrow \tau_b = \tau_a$$

and so

$$G_+ = 2\pi\tau_a \exp\left(\frac{-\Delta E}{D/\gamma}\right) \tag{5.21}$$

The calculation for G_- can be done analogously

$$\frac{G_+}{G_-} = \exp(+2\pi\Delta\omega/D) \tag{5.22}$$

For $\Delta\omega = 0$ we get

$$G_+ = G_- = \frac{\lambda}{2\pi} \exp\left(-\frac{2\lambda}{D}\right) \tag{5.23}$$

The theory can be also extended to more than two oscillators.

6 Stochastic Resonance

This is an example where noise plays a beneficial role for the detection of noisy oscillatory signals. We will consider a minimal model: Consider diffusion in a double-well potential $U_0 = -\frac{x^2}{2} + \frac{x^4}{4}$ and add weak periodic driving $U = U_0 + A\cos(\Omega t)$ as an input signal.

Consider over-damped stochastic dynamics

$$\dot{x} = -\frac{\partial U}{\partial x} + \xi, \quad \langle \xi(t)\xi(t')\rangle = 2D\delta(t-t') \tag{6.1}$$

Remember the Kramer escape rates

$$r_0 = \frac{1}{2\pi}\sqrt{|U_0''(0)|U_0''(1)}\exp\left(-\frac{\Delta U_0}{D}\right) = \frac{\sqrt{2}}{2\pi}\exp\left(-\frac{1}{4D}\right) \tag{6.2}$$

The stead-state distribution is a Boltzman distribution. Next look at the largest negative eigenvalue $\lambda_1 =\approx -r_0$, i.e. the slowest decaying mode.

We can coarse-grain the stochastic process on a two state (telegraph) process, i.e. $x \approx -1 \leftrightarrow x \approx +1$ with a time scale given by the rates ging from left to the right $r_1(n_- \to n_+)$ and back $r_2(n_- \to n_+)$ and due to particle number conservation we have $\dot{n}_+ = -\dot{n}_- = r_- n_- - r_+ n_+ = r_-(r_+ + r_-)n_+$ so e can write down a formal solution

$$n_+(t) = \exp\left(-\int_{t_0}^{t} \mathrm{d}t'\, r\right) n_+(t_0) + \exp\left(-\int_{t_0}^{t} \mathrm{d}t'\, r\right)\int_{t_0}^{t} \mathrm{d}t'\, r(t')\exp\left(\int_{t_0}^{t'} \mathrm{d}t''\, r\right) \tag{6.3}$$

So lets apply this to the case $U = U(t)$ and to simplify our life we will assume $A \ll D$

$$r_\pm 0 = \frac{\sqrt{2}}{2\pi}\exp\left(-\frac{1}{4D} \mp \frac{A}{D}\cos(\Omega t)\right) =\approx r_0\left(1 \mp \frac{A}{D}\cos(\Omega t)\right) \tag{6.4}$$

So if we insert this in the expression for n_+ we get

$$\begin{aligned} n_+(t) =& \exp(-2r_0(t-t_0))[n(t_0) + \frac{1}{2}\exp(2r_0(t-t_0) - 1) \\ &+ \frac{r_1}{\sqrt{\Omega^2 + 4r_0^2}}\cos(\Omega t - \varphi)\exp(2r_0(t-t_0) - \cos(\Omega t - \varphi))] \end{aligned}$$

with $r_1 = \frac{r_0 A}{D}$ and $\tan(\varphi) = \frac{\Omega}{2r_0}$ and for $t \gg t_0$ we get

$$n_+ = \frac{1}{2} + \frac{r_1}{\sqrt{\Omega^2 + 4r_0^2}} \cos(\Omega t - \varphi) \tag{6.5}$$

Next we look at the autocorrelation function of this process

$$\langle x(t) \rangle = x_+ p_+(t) + x_- p_-(t) = p_+(t) - p_-(t) \tag{6.6}$$

with $x_\pm = \pm 1$ and $p_+ = n_+/n$ and so we get

$$\begin{aligned} \langle x(t)x(t+\tau)|x_0, t_0\rangle &= \sum_{s,s'} s \cdot s' P(s, t+\tau|s', t) P(s', t|x_0, t_0) \\ &= p_+(t+\tau| + 1, t) p_+(+1, t|x_0, t_o) + \ldots \end{aligned}$$

(take all combinations $11, 1-1, -11, -1-1$)

We use $p_p = 1 - p_+$ and consider the limit $t_0 \to -\infty$, thus

$$\begin{aligned} \langle x(t)x(t+\tau)\rangle =& \exp(-2r_0\tau) + 2r_1 \\ &+ 4r_1^2[\exp(-2r_0\tau)\cos^2(\Omega t - \varphi) + \cos(\Omega(t+\tau) - \varphi)\cos(\Omega t - \varphi)] \end{aligned}$$

Now the autocorrelation function depends on time, as this is not just a static process, i.e. time translation symmetry is broken. Note that is only depends on $\Omega t \% 2\pi$, so it doesn't matter which cycle of driving is chosen.

If we average over t we get

$$C(\tau) = \langle x(t)x(t+\tau)\rangle_t = \exp(-2r_0|\tau|)[1 - 2r_1^2] + 2r_1^2 \cos(\Omega t) \tag{6.7}$$

with a decaying and periodic component. We get the power spectral density be doing a Fourier transform by the Wiener-Klinchine theorem

$$S(\omega) = F(C(\tau)) = (1 - 2r_1^2)\frac{4r_0}{4r_0^2 + \omega^2} + 2\pi r_1^2(\delta(\omega - \Omega) + \delta(\omega + \Omega)) \tag{6.8}$$

The first term determines the noise contribution (decaying term / a Lorentzian) and the

second term represents the periodic contribution. So one defines the signal-to-noise ration

$$SNR = \frac{S}{B} = \pi \frac{r_1^2}{r_0} = \frac{1}{\sqrt{2}} \frac{A^2}{D^2} \exp\left(-\frac{1}{4D}\right) \tag{6.9}$$

So our signal is better, if we have some noise in our system! The SNR attains a maximum at a finite D (before the decay with D^{-2}). This can be intuitively understood that for $\frac{1}{r} = \frac{1}{2}T = \frac{1}{2}\frac{2\pi}{\Omega}$ then the particle is jumping according to the oscillatory change in the potential.

Glimpse on Infotaxis: Infotaxis as a strategy for searching without gradients by Vergassola 2007

7 Itō versus Stratonovich Calculus

If we are given an ODE, e.g. $\dot{x} = f(x)$, what does this mean? To answer this question, we are going to take a constructive approach and interpret the ODE as a rule to construct the solution. So we estimate the values $x_i = x(i\,\mathrm{d}t)$ and then take the limit $\mathrm{d}t \to 0$.

7.1 Numerical Motivation

Deterministic ODE

For a deterministic ODE, we have various options to chose a scheme in order to solve them numerically. One could use either an explicit scheme like the Euler scheme

$$x_i = x_{i-1} + f(x_{i-1})\,\mathrm{d}t \tag{7.1}$$

and implicit scheme

$$x_i = x_{i-1} + f(x_i)\,\mathrm{d}t \tag{7.2}$$

or a mixed scheme

$$x_i = x_{i-1} + \frac{1}{2}[f(x_{i-1}) + f(x_i)] \tag{7.3}$$

and all schemes will converge to the same limit.

Stochastic Differential Equations

Also for stochastic differential equations, such as $\dot{x} = f(x) + \sqrt{2D(x)}\xi$, we may chose either an explicit scheme (Itō)

$$x_i = x_{i-1} + f(x_{i-1})\,\mathrm{d}t + \sqrt{2D(x_{i-1})}N_i\sqrt{\mathrm{d}t} \tag{7.4}$$

with $N_i \in N(0,1)$. Alternatively, we could consider a mixed scheme (Stratonovich)

$$x_i = x_{i-1} + \frac{1}{2}[f(x_{i-1}) + f(x_i)]\,\mathrm{d}t + \frac{1}{2}[\sqrt{2D(x_{i-1})} + \sqrt{2D(x_i)}]N_i\sqrt{\mathrm{d}t} \tag{7.5}$$

It is important to note that this time both schemes are different. (A purely implicit scheme for SDE is not discussed, because such schemes are rarely used in practice.) We can see this by doing the expansion

$$x_i = x_{i-1} + f(x_{i-1})\,\mathrm{d}t + \mathcal{O}(\mathrm{d}t^{3/2}) + g(x_{i-1})N_i\sqrt{\mathrm{d}t} + g'(x_{i-1})g(x_{i-1})N_i^2\,\mathrm{d}t \tag{7.6}$$

with $\langle N_i^2 \rangle = 1$, so that the last term can not be neglected!

7.2 Different Interpretations

Having a look at the chain rule, one can see that the Itō and Stratonovich interpretation are indeed two different sorts of calculus. In Stratonovich interpretation the ordinary chain rule holds

$$\text{(S)} \quad y = y(x), \quad \dot{y} = \frac{\partial y}{\partial x}\dot{x} \tag{7.7}$$

By contrast, in Itō interpretation we have $\dot{x}_k = f_k + g_{kl}\xi_l$ with $\langle \xi_k(t)\xi_l(t') \rangle = \delta_{kl}\delta(t-t')$ and the Itō chain rule applies

$$\text{(I)} \quad y = y(x), \quad \dot{y} = \frac{\partial y}{\partial x_j}\dot{x}_j + \frac{1}{2}\frac{\partial^2 y}{\partial x_k \partial x_l}g_{km}g_{ml} \tag{7.8}$$

Switching between Itō and Stratonovich

We consider the same stochastic dynamic $x(t)$ represented by a Langevin equation in either Itō or Stratonovich calculus.

In Itō and Stratonovich calculus, respectively, we have

$$\begin{aligned} \text{(S)} \quad & \dot{x}_k = h_k^S + g_{kl}\xi_l \\ \text{(I)} \quad & \dot{x}_k = h_k^I + g_{kl}\xi_l \end{aligned}$$

with $h_k^I = h_k^S + \frac{1}{2}\frac{\partial g_{kl}}{\partial x_m} g_{ml}$. The Fokker Planck Equation reads for these cases

$$\dot{P} = \frac{\partial}{\partial x_k}\left[-\left(h_k^{I/S} + \alpha \frac{\partial g_{kl}}{\partial x_m} g_{ml}\right) P + \frac{1}{2}\frac{\partial}{\partial x_m}\left(g_{kl} g_{ml} P\right)\right] \tag{7.9}$$

with $\alpha = 0$ for Itō and $\alpha = 1/2$ for Stratonovich calculus.

> **Wong-Zakai Theorem**
>
> If $\dot{x} = f(x) + g(x)\xi$ is a SDE with coloured noise of finite correlation τ, then taking the limit $\tau \to 0$ yields a Stratonovich SDE with Gaussian white noise.

Example of Colored Noise (Ornstein-Uhlenberg process)

$\tau\dot{\xi} = -\xi + \eta$ and $\langle \eta(t)\eta(t')\rangle = \delta(t-t') \Rightarrow \langle \eta(t)\eta(t')\rangle \sim \exp\left(-\frac{-|t-t'|}{\tau}\right)$

Toy example I: Geometric Brownian Motion

We consider the example of (I) $\dot{x} = x\xi$ (*), which corresponds to (S) $\dot{x} = x\xi - Dx$. Now we ask about the time evolution of the first moment $m(t) = \langle x(t)\rangle$? In Itō calculus, we have

$$\frac{\mathrm{d}}{\mathrm{d}t} m(t) = \langle \dot{x}\rangle \overset{(I)}{=} \langle x\xi\rangle = \langle x\rangle \underbrace{\langle \xi\rangle}_{=0} = 0 \tag{7.10}$$

so $m(t) = m_0$. Note that $y = \ln(x) \Rightarrow \dot{y} = \xi - D \Rightarrow y(t) \sim N(-Dt, Dt)$

Toy example II

Next, let's do something forbidden and literally read the Itō SDE (*) as Stratonovich SDE (S) $\dot{x} = x\xi$. This Stratonovich SDE would actually correspond to the Itō SDE (I) $\dot{x} = x\xi + Dx$. Now

$$\frac{\mathrm{d}}{\mathrm{d}t} m(t) = \langle \dot{x}\rangle \overset{(I)}{=} \langle x\xi + Dx\rangle = 0 + Dm \tag{7.11}$$

hence, in Itō calculus this time we get $m = m_0 \exp(Dt)$.

Example: Rotational diffusion in 2D

We have for the stochastic dynamics of the azimuthal angle $\dot{\varphi} = \xi$. For the dynamics of the material frame vectors

$$\vec{e}_1 = \begin{pmatrix} \cos(\varphi) \\ \sin(\varphi) \end{pmatrix}, \quad \vec{e}_2 = \begin{pmatrix} -\sin(\varphi) \\ \cos(\varphi) \end{pmatrix}$$

we have

$$\text{(S)} \quad \dot{e}_1 = \xi \vec{e}_2, \quad \dot{e}_2 = \xi \vec{e}_1 \tag{7.12}$$

In order to rewrite the SDE in Itō interpretation we introduce

$$\vec{e}_1 = \begin{pmatrix} x_1 \\ x_2 \end{pmatrix}, \quad \vec{e}_2 = \begin{pmatrix} x_3 \\ x_4 \end{pmatrix}$$

with

$$\dot{\vec{x}} = \vec{g}\xi, \quad \vec{g} = (x_3 x_4 - x_1 - x_2)^T$$

and with $\sum_m \frac{\partial g_k}{\partial x_m} g_m = 2D(-\vec{x})$, we find

$$\text{(I)} \quad \dot{e}_1 = \xi \vec{e}_2 - D\vec{e}_1, \quad \dot{e}_2 = \xi \vec{e}_1 - D\vec{e}_2 \tag{7.13}$$

Extended Example: persistent random walk (2D)

Consider $\vec{r} = v_0 \vec{e}_1$ where $(\vec{e}_1, \vec{e}_2)$ is subject to rotational diffusion. Our proposition is that

$$C(t) = \langle \vec{e}_1(t) \cdot \vec{e}_1(t) \rangle = \exp(-Dt) \tag{7.14}$$

with persistence time $t_p = \frac{1}{D}$ and persistence length $l_p = v_0 t_p$.

Proof: $\frac{\mathrm{d}}{\mathrm{d}t} C(t) = \left\langle \vec{e}_1(t) \cdot \dot{\vec{e}}_1(t) \right\rangle = \vec{e}_1(t) \cdot [\xi \vec{e}_2(t) - D\vec{e}_1(t)] = 0 - D$

7.3 Rotational Diffusion in 3D

As another example we consider rotational diffusion in 3D with the rotational diffusion coefficient (instance of the Fluctuation-Dissipation-Theorem!)

$$D_{\text{rot}} = \frac{k_B T}{8\pi\eta r^3} \tag{7.15}$$

and the parameterization

$$\begin{aligned}
\vec{h}_3 &= (\cos(\psi), \sin(\psi)\cos(\vartheta), \sin(\psi)\sin(\vartheta))^T \\
\vec{g}_1 &= -\frac{\partial \vec{h}_3}{\partial \psi} \quad \vec{g}_2 = -\vec{h}_3 \times \vec{g}_1 \\
\vec{h}_1 &= \cos(\varphi)\vec{g}_1 + \sin(\varphi)\vec{g}_2 \quad \vec{h}_2 = \vec{h}_3 \times \vec{h}_1
\end{aligned}$$

The equations of motion are given by the Frenet-Serret equations for Stratonovich calculus

$$(S) \quad \begin{aligned}
\dot{\vec{h}}_3 &= \xi_2 \vec{h}_1 - \xi_1 \vec{h}_2 \\
\dot{\vec{h}}_1 &= \xi_3 \vec{h}_2 - \xi_2 \vec{h}_3 \\
\dot{\vec{h}}_2 &= \xi_1 \vec{h}_3 - \xi_3 \vec{h}_1
\end{aligned}$$

with $\langle \xi_i(t)\xi_j(t')\rangle = \delta_{i,j}\delta(t-t')2D_{\text{rot}}$ and

$$(\text{S}) \quad \dot{\psi} = \sin(\varphi)\xi_1 + \cos(\varphi)\xi_2 \tag{7.16}$$

which is equivalent to

$$(\text{I}) \quad \dot{\psi} = \underbrace{\sin(\varphi)\xi_1 + \cos(\varphi)\xi_2}_{=\xi(t)} + D_{\text{rot}}\cot(\psi) \tag{7.17}$$

in Ito calculus. We can replace the multiplicative noise term by $\xi(t)$ because

$$\begin{aligned}
\langle \xi(t)\xi(t')\rangle &= \langle [\sin(\varphi(t))\xi_1 + \cos(\varphi(t))\xi_2][\sin(\varphi(t'))\xi_1 + \cos(\varphi(t'))\xi_2]\rangle \\
&= \sin(\varphi(t))\sin(\varphi(t'))\langle \xi_1(t)\xi_1(t')\rangle + \cos(\varphi(t))\cos(\varphi(t'))\langle \xi_2(t)\xi_2(t')\rangle \\
&= [\sin^2(\varphi) + \cos^2(\varphi)]2D_{\text{rot}}\delta(t-t') = 2D_{\text{rot}}\delta(t-t')
\end{aligned}$$

We know that the steady-state distribution must be isotropic, so let's check this. The question is, what is $P^*(\psi)$ for isotropic distribution of $\vec{h}_3$? We have the height $h = 1 - \cos(\psi)$, so $A = 2\pi r h$, $\mathrm{d}A = 2\pi\,\mathrm{d}h$. Thus $P^*(h) = \frac{1}{2}$. Furthermore, $P^*(h)\,\mathrm{d}h = P^*(\psi)\,\mathrm{d}\psi$ with $\mathrm{d}h = \sin(\psi)\,\mathrm{d}\psi$ and so $P^*(h) = \frac{1}{2}\sin(\psi)$

The equation of motion can be also rewritten introducing a potential U

$$\text{(I)} \quad \dot{\psi} = D_{\mathrm{rot}}\cot(\psi) + \xi = -\frac{1}{\gamma}\frac{\partial}{\partial\psi}U + \xi \tag{7.18}$$

with $U = -D_{\mathrm{rot}}\gamma\ln(\sin(\psi)) = k_B T\ln(\sin(\psi))$ and $\gamma = 8\pi\eta r^3$. Thus,

$$P^*(\psi) \sim \exp\left(-\frac{U}{k_B T}\right) \sim \exp(\ln(\sin(\psi))) \sim \sin(\psi) \tag{7.19}$$

An Interpretation of $U(\psi)$ is obtained by taking a look at the entropy $S = k_B\ln(\sin(\psi))$ and the free energy $F = -TS = -D_{\mathrm{rot}}\gamma\ln(\sin(\psi)) = U$. Here, knowing $\vec{h}_3$ corresponds to the microstate and knowing h to the macro state.

7.4 How to derive a correct Langevin equation?

1) can be considered as a limit case of coloured noise $\tau_c \to 0$, then employ Wong-Zakai-theorem

2) small number fluctuations (e.g. for chemical reactions, so suppose you have N particles which can transit from 1 to 2 with rate r_2 and from 2 to 1 with rate r_1, so one can derive a continuum limit of a master equation)

3) only thermal fluctuations $T = \text{const}$ and then use $P^* \sim \exp(-\beta U)$

Master Equation for a Two-State System

Let $P(n)$ be the probability, that n entities are in state 2. Then, the Dynamic equation / Master equation for $P(n)$ is given by

$$\begin{aligned}\dot{P}(n,t) &= r_1(n+1)P(n+1,t) - r_1 nP(n,t) + r_2(N-(n-1))P(n-1,t) - r_2(N-n)P(n,t)\\ &= r_1(E^+ - 1)nP + r_2(E^- - 1)(N-n)P\end{aligned}$$

with the shift operators $E^{\pm}$

$$(E^{+}f)(n) = f(n+1) \quad \text{and} \quad (E^{-}f)(n) = f(n-1)$$

In order to go to a continuum limit we let $x = \frac{n}{N}$ and treat x as a continuous variable. Next, we do a Taylor expansion of our fancy step operators

$$(E^{\pm}f)(x) = f(x \pm \frac{1}{N}) = f(x) \pm f'(x)\frac{1}{N} + \frac{1}{2}f''(x)\frac{1}{N^2} + \dots$$

which we feed back so that we get

$$\begin{aligned}\dot{P}(x,t) &= r_1\frac{\partial}{\partial x}(xP) + \frac{r_1}{2N}\frac{\partial^2}{\partial x^2}(xP) - r_2\frac{\partial}{\partial x}[(1-x)P] + \frac{r_2}{2N}\frac{\partial^2}{\partial x^2}[(1-x)P] \\ &= (r_1+r_2)\frac{\partial}{\partial x}[(x-x^*)P] + \frac{1}{2N}\frac{\partial^2}{\partial x^2}[(r_1+(r_1-r_2)x)P]\end{aligned}$$

with $x^* = \frac{r_2}{r_1+r_2}$. In the steady state we have $r_0 = r_1 = r_2$ and the master equation $\dot{P} = -\vec{\nabla}J$ with $J = 0$ at equilibrium, thus $P^*(x) \sim \exp\left(-\frac{(x-\frac{1}{2})^2}{2\sigma^2}\right)$ and $\sigma^2 = \frac{1}{4N}$

Langevin equation

$$\text{(I)} \quad \dot{x} = (r_1+r_2)(x^*-x) + \underbrace{\sqrt{\frac{r_1x + r_2(1-x)}{2N}}}_{=g(x)}\xi \tag{7.20}$$

$$\text{(S)} \quad \dot{x} = (r_1+r_2)(x^*-x) + \underbrace{\sqrt{\frac{r_1x + r_2(1-x)}{2N}}}_{=g(x)}\xi - \frac{1}{2}\frac{r_1-r_2}{4N} \tag{7.21}$$

In the limit $N \gg 1$ we have $x \approx x^*$. Thus, $g(x) \approx g(x^*)$ and $P^*(x) = N(x^*, \sigma^2)$, $\sigma^2 = \frac{1}{N}\frac{r_1r_2}{(r_1+r_2)^2}$.

7.5 Numerical Integration of nonlinear SDE

To numerically integrate an Itō SDE (I) $\dot{x} = f(x) + g(x)\xi(t)$, $\langle \xi(t)\xi(t') \rangle = \delta(t - t')$, we can use the Euler-Maruyama scheme

$$\begin{aligned} x_{t+\Delta t} &= x_t + f(x_t)\Delta t + g(x_t)N_t, & N_t &\sim N(0, \Delta t) \\ x_{t+\Delta t} &= x_t + f(x_t)\Delta t + g(x_t)N'_t\sqrt{\mathrm{d}t}, & N'_t &\sim N(0, 1) \end{aligned}$$

For the integration of an Stratonovich SDE (S) $\dot{x} = f(x) + g(x)\xi(t)$ we can use the Euler-Heun scheme

$$x_{t+\Delta t} = x_t + f(x_t)\Delta t + \tfrac{1}{2}[g(x_t) + g(\bar{x}_t)]N_t, \qquad N_t \sim N(0, 1)$$

where $\bar{x}_t = x_t + g(x_t)N_t$

8 Fluctuation-Dissipation-Theorem

8.1 Historical Examples

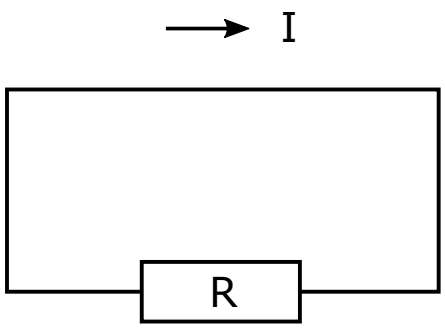
Example 1: Diffusion (Einstein 1905)

The relation found be Einstein for ordinary diffusion in 1905

$$D = \frac{k_B T}{\gamma} \tag{8.1}$$

is an instance of the fluctuation dissipation theorem. The diffusion coefficient D characterises the mean square displacement $\langle x^2(t)\rangle = 2Dt$ (fluctuations) and the right-hand side is related to the dissipated energy via the hydrodynamic mobility $\frac{1}{\gamma} = \frac{1}{6\pi\eta a}$ so that the velocity is given by $v = \frac{1}{\gamma}F$.

Example 2: Electrothermal noise (Johnson, Nyquist 1927)

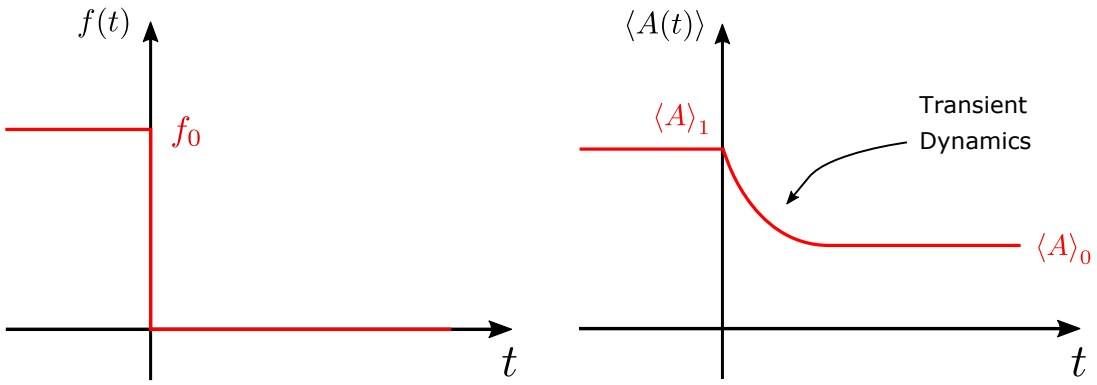


It was found that even a shorted circuit consisting of just one resistor does show a finite current, which is zero on average $\langle I\rangle = 0$, but has a non-zero fluctuation spectrum

$$S_I^{(\omega)} = 2\frac{k_B T}{R\pi} \tag{8.2}$$

Here, we assume the classical limit $\hbar\omega \ll k_B T$. The inverse resistance plays the role of a linear response coefficient $I = \frac{1}{R}U$.

8.2 FDT for classical systems



Lets consider a system described by the Hamiltonian $H_1 = H_0 - fA$ for times $t < 0$, with the probability density $p_1(x) \sim \exp(-\beta H_1)$. At $t = 0$ we switch off the external field f coupled to the observable A. Thus, $p(x,t) \to \exp(-\beta H_0)$ for $t \to \infty$. The ensemble-average of A is given by $\langle A\rangle = \int \mathrm{d}x\, A(x)p(x,t)$ and we integrate over microstates $x = (p_1, \ldots, p_N, q_1, \ldots, q_N)$.

> **Fluctuation Dissipation Theorem**
>
> The FDT relates the fluctuation spectrum on the left side to the dissipative response to an external field on the right side of
>
> $$S_A(\omega) = \frac{2k_BT}{\omega}\,\mathrm{Im}(\tilde{\chi}_A(\omega)) \tag{8.3}$$

In order to show that the Fluctuation Dissipation Theorem holds we need to key concepts:

- Boltzman distribution $p_0 \sim \exp(-\beta H_0)$ with $\beta = \frac{1}{k_BT}$
- time propagator $P(x_1, t_1|x_0, t_0)$

Fluctuation Spectrum

The auto-correlation function is given by

$$C_A(\tau) = \langle A(t)A(t+\tau)\rangle - \langle A\rangle^2 \tag{8.4}$$

which is independent of t at thermal equilibrium. The correlation function is an even function $C_A(\tau) = C_A(-\tau)$. It is related to the time propagator by

$$C_A(\tau) = \int \mathrm{d}x_0\, \mathrm{d}x_1\, A(x_0)A(x_1)p_0(x_0)P(x_1, t+\tau|x_0, t) - \langle A\rangle^2 \tag{8.5}$$

The power spectral density is then the Fourier transform

$$S_A(\omega) = \tilde{C}_A(\omega) = \int \mathrm{d}\tau\, C_A(\tau)e^{i\omega\tau} \tag{8.6}$$

where we use the non-unitary Fourier transform with angular frequency.

> **Wiener-Kinchin Theorem**
>
> The Fourier transform exists and has the usual properties.

Formally, we have $\left\langle \tilde{A}(\omega)\tilde{A}^*(\omega')\right\rangle = S_A(\omega)\delta(\omega-\omega')$. Note, however that $\tilde{A}(\omega)$ is not in a strict mathematical sense defined.

Linear Response Function

Let a system possess the Hamiltonian $H(x,t) = H_0(x) - A(x)f(t)$. Then, the linear response is expressed by

$$\langle A(t)\rangle = \langle A\rangle_0 + \int_{-\infty}^{\infty} \mathrm{d}\tau\, \chi_A(\tau)f(t-\tau) + \mathcal{O}(f^2) \tag{8.7}$$

which defines the linear response function $\chi_A(\tau)$. Causality implies that $\chi_A(\tau) = 0$ for all $\tau < 0$.

The Fourier transform reads

$$\tilde{\chi}_A(\omega) = \int_{-\infty}^{\infty} \mathrm{d}\tau\, \chi_A(\tau)e^{i\omega\tau} \tag{8.8}$$

Example: Oscillating Field

$$f(t) = f_0 \cos(\omega t) = \operatorname{Re} f_0 e^{i\omega t} \tag{8.9}$$

then

$$\langle A(t)\rangle = \langle A\rangle_0 + [\operatorname{Re}\tilde{\chi}_A(\omega)] f_0 \cos(\omega t) - [\operatorname{Im}\tilde{\chi}_A(\omega)] f_0 \sin(\omega t) \tag{8.10}$$

so $f(t)$ oscillates with the frequency of driving with amplitude $f_0|\tilde{\chi_A}(\omega)|$ and with phase lag $\arg(\tilde{\chi_A}(\omega))$. The power performed by the external field is given by $R = -f(t)\frac{\mathrm{d}}{\mathrm{d}t}A(x(t))$ with the time-average $\langle R\rangle = \frac{1}{2}\omega f_0^2 \operatorname{Im}\tilde{\chi_A}(\omega)$. Thus, the imaginary part $\operatorname{Im}\tilde{\chi}_A(\omega)$ characterises the dissipative response of the system.

Derivation of the fluctuation-dissipation-theorem

Let $f(t) = f_0\Theta(-t)$. We first compute the partition function $Z_1 = \int \mathrm{d}x \exp\{-\beta H_1\}$ with

$$f_1(x) = \frac{1}{Z_1}\exp\{-\beta H_1\} \approx p_0(x)[1 + \beta f_0(A(x) - \langle A\rangle_0)] \tag{8.11}$$

For $t \geq 0$ we have

$$\begin{aligned}
\langle A(t)\rangle &= \int \mathrm{d}x\, A(x)p(x,t) = \int \mathrm{d}x\, A(x) \int \mathrm{d}x_0\, P(x,t|x_0,t_0)p_1(x_0) \\
&= \int \mathrm{d}x\, A(x) \int \mathrm{d}x_0\, P(x,t|x_0,t_0)p_0(x_0)[1 + \beta f_0 A(x) - \beta f_0 \langle A\rangle_0] \\
&= \langle A\rangle_0 + \beta f_0 \langle A(t)A(0)\rangle - \beta f_0 \langle A\rangle_0^2 \\
&= \langle A\rangle_0 + \beta f_0 C_A(t)
\end{aligned}$$

We also know that

$$\langle A(t)\rangle = \langle A\rangle_0 + \int_{-\infty}^{\infty} \mathrm{d}\tau\, \chi_A(\tau) f(t-\tau) \tag{8.12}$$

The derivative with respect to time reads

$$\chi_A(t) = \begin{cases} \beta \frac{\mathrm{d}}{\mathrm{d}t} C_A(t) & for \quad t \geq 0 \\ 0 & for \quad t < 0 \end{cases}$$

Remark: Even and Odd Functions

Every function $F(t)$ can be separated into an even and an odd part

$$F(t) = \begin{cases} F'(t) = \frac{1}{2}[F(t) + F(-t)] \,(\text{even}) & \Rightarrow \quad \tilde{F}'(\omega) = \operatorname{Re} \tilde{F}(\omega) \\ F''(t) = \frac{1}{2}[F(t) - F(-t)] \,(\text{odd}) & \Rightarrow \quad \tilde{F}'(\omega) = i \operatorname{Im} \tilde{F}(\omega) \end{cases}$$

Caution: The prime $'$ indicates the even part, not a derivative!

so $C_A(t)$ is even, thus $\frac{\mathrm{d}}{\mathrm{d}t} C_A(t)$ is odd and as we take only the odd parts $\chi''_A(t) = \frac{1}{2}\beta \frac{\mathrm{d}}{\mathrm{d}t} C_A(t)$ and so $i \operatorname{Im} \tilde{\chi}_A(\omega) = \frac{1}{2}\beta(+i\omega)\delta_A(\omega)$

In classical mechanics we have $\frac{1}{\beta} = k_B T$, in quantum mechanics we have $\hbar\omega = \coth \frac{\beta\hbar\omega}{2}$

Example: Optical Trap

An optical trap can be described by

$$kx + \gamma\dot{x} = \gamma\xi(t) \quad \text{with} \quad \langle \xi(t) \rangle = 0 \tag{8.13}$$

The fluctuation dissipation theorem is telling us that

$$S_x(\omega) = \frac{2k_B T}{\omega} \operatorname{Im} \tilde{\chi}_x(\omega) = \frac{2k_B T/\gamma}{(k/\gamma)^2 + \omega^2} \tag{8.14}$$

Thus, one can estimate k by measuring $S_x(\omega)$. As a generalised example, we consider

$$\sum_{k=0}^{n} a_k x^{(k)}(t) = \xi(t) \tag{8.15}$$

for which we do a a Fourier transformation in order to get

$$\underbrace{\sum_{k=0}^{n} a_k (i\omega)^k}_{=\tilde{\chi}_A^{-1}(\omega)} \tilde{\chi}(\omega) = \tilde{\xi}(\omega) \tag{8.16}$$

so

$$\begin{aligned}\tilde{\chi}(t) &= \tilde{\chi}_A(t)\tilde{\xi}(\omega) \\ \chi(t) &= \int_0^\infty \mathrm{d}\tau\, \tilde{\chi_A}(\tau)\xi(t-\tau)\end{aligned}$$

We have

$$\begin{aligned}S_x(\omega)\delta(\omega-\omega') &= \langle \tilde{\chi}(\omega)\tilde{\chi}^*(\omega')\rangle \\ &= \tilde{\chi}_A(\omega)\tilde{\chi}_A^*(\omega')\left\langle \tilde{\xi}(\omega)\tilde{\xi}(\omega')\right\rangle \\ &= |\tilde{\chi}_A(\omega)|^2 2D\delta(\omega-\omega')\end{aligned}$$

so

$$S_x(\omega) = |\tilde{\chi}_A(\omega)|^2 2D = \frac{2k_BT}{\omega}\,\mathrm{Im}\,\tilde{\chi}_A(\omega) \tag{8.17}$$

$$2D = \frac{2k_BT}{\omega}\frac{\mathrm{Im}\,\tilde{\chi}_A(\omega)}{|\tilde{\chi}_A(\omega)|^2} \tag{8.18}$$

For the special case $a_1 = \gamma$, but $(a_{2k+1} = 0)$ for $k > 0$ we have

$$\tilde{\chi}_A = \frac{1}{R(\omega) - i\omega\gamma} \quad \Rightarrow \quad \mathrm{Im}\,\tilde{\chi}_A = \frac{\omega\gamma}{R^2(\omega) + \omega^2\gamma^2} \tag{8.19}$$

Thus, $D = k_BT\gamma$

9 A Link to Statistical Physics

The fluctuation-dissipation theorem is a hallmark of equilibrium systems. Living systems can violate the fluctuation-dissipation theorem.

9.1 Detailed Balance

A system that can reach equilibrium andhas a zero net current at equilibrium obeys to so-called detailed balance. It means, that it is not possible to distinguish whether a dynamics is played forwards or backwards in time. It defines reversible Markov chains.

We can formulate the condition of detailed balance both for continuous and discrete state space descriptions.

Condition for Detailed Balance

We say the dynamics obeys "detailed balance" if

- there exists an equilibrium distribution P^* or P_j^* in the discrete case
- the joint probability is symmetric $P^*(x', \tau|x, 0) = P^*(x, \tau|x', 0)$ and $P^*(i, \tau|j, 0) = P^*(j, \tau|i, 0)$ / $L_{ji}P_j^* = L_{i,j}P_i^*$, respectively

Its behaviour is governed for continuous state space by the Fokker-Planck equation

$$\frac{\mathrm{d}}{\mathrm{d}t}p(x,t) = \hat{L}p(x,t) \tag{9.1}$$

and for discrete state space by the Master equation

$$\frac{\mathrm{d}}{\mathrm{d}t}P_j(t) = P_i(t)L_{ij} \tag{9.2}$$

This means that there is zero net current at equilibrium $i \rightleftharpoons j$. So for example if the transition matrix is symmetric a system obeys detailed balance.

Example: Boltzmann distribution

A simple example is the Boltzmann distribution for a canonical ensemble, where you have states $0, 1, 2, \ldots$ with energies $E_0, E_1, E_2, \ldots$ so

$$P_i^* = \frac{1}{Z} \exp(-\beta E_i) \tag{9.3}$$

and

$$\frac{L_{ji}}{L_{ij}} = \exp(-\beta(E_i - E_j)) \tag{9.4}$$

A counter example would be a circular current $1 \to 2 \to 3 \to 1$ with rate r giving

$$\hat{L} = \begin{pmatrix} -r & r & 0 \\ 0 & -r & r \\ r & 0 & -r \end{pmatrix} \tag{9.5}$$

with eigenvalue $\lambda_1 = 0$ with corresponding eigenvector $\vec{e}_1 = \left(\frac{1}{3}, \frac{1}{3}, \frac{1}{3}\right)^T$ and $\lambda_2 = \lambda_3^* = \left(-\frac{3}{2} + i\frac{\sqrt{3}}{2}\right) r$ resulting in a net current at equilibrium, thus breaking detailed balance.

Proof of Detailed Balance for Hamiltonian Systems

We consider a system characterised by some Hamiltonian H obeying the Hamilton equations

$$\dot{p}_i = -\frac{\partial H}{\partial q_i} \quad \dot{q}_i = \frac{\partial H}{\partial p_i} \tag{9.6}$$

with the macroscopic observable $y = Y(q, p)$. The detailed balance holds if

(i) H is even in p_i

(ii) Y is even in p_i

Then the time propagator T fulfills the condition

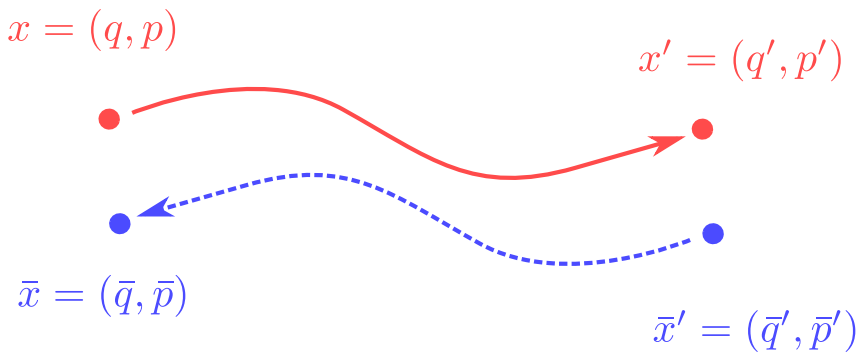
$$P(y', \tau|y, 0) = T_\tau(y'|y)P^*(y) = T_\tau(y|y')P^*(y') = P(y, \tau|y', 0) \tag{9.7}$$

Nota Bene

We always have

$$T_\tau(y'|y)P^*(y) = T_{-\tau}(y|y')P^*(y) \tag{9.8}$$

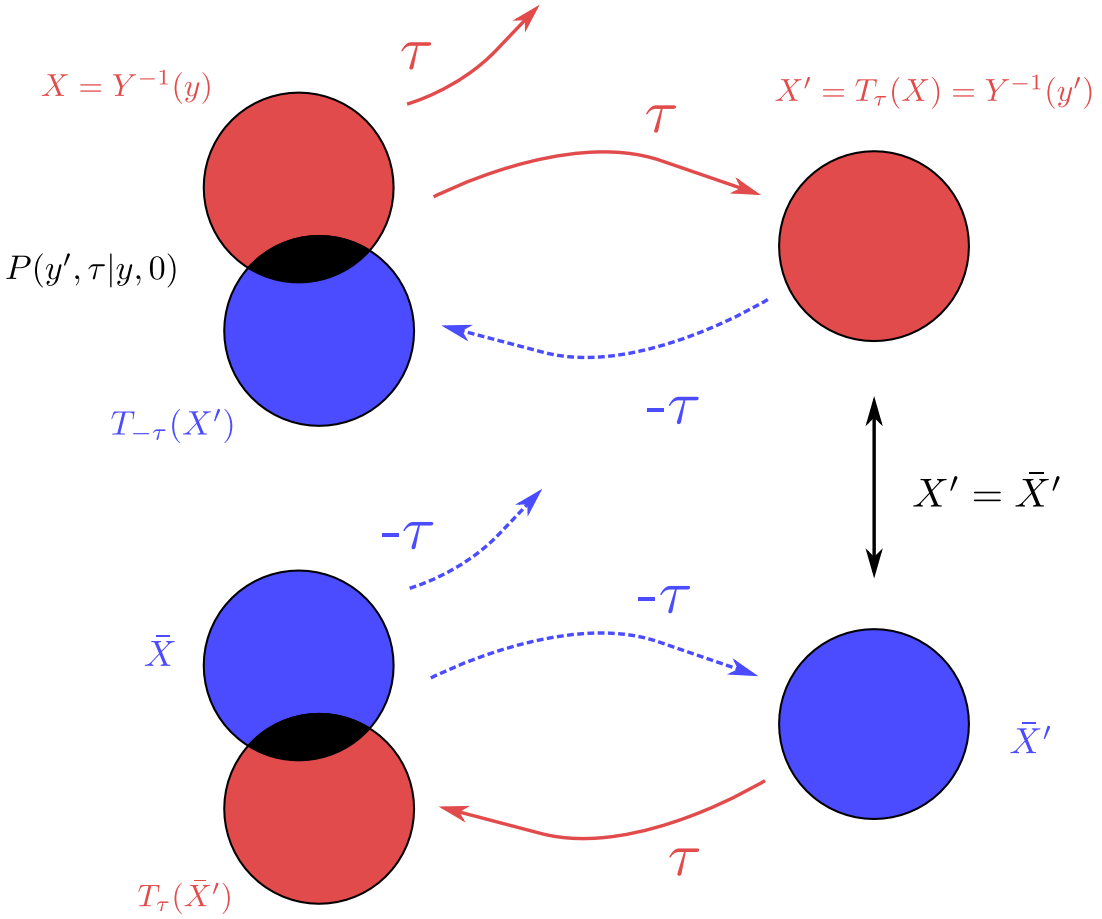
as we can play backwards the dynamics in time.



For the proof of this we make use of time reversal notation

$$\bar{t} = -t \quad \bar{q}_i = q_i \quad \bar{p}_i = -p_i \tag{9.9}$$

We start by looking at a trajectory in (q, p)-phase space and for every point $x' = (q', p')$ we apply time reversal $\bar{x}' = (\bar{q}', \bar{p}')$. By (i) we conclude that $H(x) = H(\bar{x})$ and thus $P^*(x) = P^*(\bar{x})$ (even in p_i means in our case symmetric in time!). Also, we have $X = Y^{-1}(y)$ and by (ii) $X = \bar{X}$ as Y is even.



We can express the probability to observe y' at time τ after observing y at time 0 by the integral over the phase space region $X \cap T_{-\tau}(X')$ of the equilibrium probabilities $P^*(x)$

$$T_\tau(y'|y)P^*(y) = P(y', \tau|y, 0) = \int_{X \cap T_{-\tau}(X')} \mathrm{d}x \, P^*(x)$$

As we have $P^*(x) = P^*(\bar{x})$ we can also change the area of integration in phase space to $\overline{X \cap T_{-\tau}(X')}$

$$\int_{X \cap T_{-\tau}(X')} \mathrm{d}x \, P^*(x) = \int_{\overline{X \cap T_{-\tau}(X')}} \mathrm{d}x \, P^*(x)$$

From the diagram above we see that the states in the lower red circle $T_\tau(\bar{X}')$ are mapped to the states in the upper blue circle $T_{-\tau}(X')$ under time reversal

$$\overline{T_{-\tau}(X')} = T_\tau(\bar{X}') \tag{9.10}$$

and so we have

$$\overline{X \cap T_{-\tau}(X')} = \bar{X} \cap \overline{T_{-\tau}(X')} = \bar{X} \cap T_\tau(\bar{X}') = X \cap T_\tau(X') \tag{9.11}$$

We conclude

$$\int_{\overline{X \cap T_{-\tau}(X')}} \mathrm{d}x\, P^*(x) = \int_{X \cap T_\tau(X')} \mathrm{d}x\, P^*(x) = P(y, \tau | y', 0) = T_\tau(y|y') P^*(y') \tag{9.12}$$

So at equilibrium we cannot distinguish whether a dynamics is played forward or backward in time.

9.2 Increase of Relative Entropy

We consider a Master equation for a Markov chain

$$P_j^{(n+1)} = \sum_i P_i^n\, T_{ij} \tag{9.13}$$

with the probability P_i^n to be in state i at time $t = t_n$ and a matrix of transition probabilities (T_{ij}) fulfilling $\sum T_{ij} = 1$. For a stationary distribution with $P_j^* > 0$ so that $P_j^* = \sum_i P_i^*\, T_{ij}$ for all j, we define the relative entropy (Kullberg-Leibler divergence) as

$$D_n = KL(P^n || P^{-k}) = \sum P_i^n \ln\left(\frac{P_i^n}{P_i^*}\right) \tag{9.14}$$

> **Theorem**
>
> $D_{n+1} \leq D_n$

This theorem is a direct consequence of the convexity of D_n. For $P_i^* = \frac{1}{N}$, one finds that $D_n = -\sum P_i \ln(P_i) - \ln(N)$, i.e. the entropy increases with time.

9.3 Equilibrium vs Non-Equilibrium

Signs of Equilibrium

- FDT
- detailed balance $L_{ji}P_j^* = L_{ij}P_i^*$
- equipartition theorem

All of these constrain the Langevin equation to approach thermal equilibrium. At equilibrium we have the Boltzmann distribution as a maximum entropy distribution.

Let us consider a macrostate y with microstates $x = Y^{-1}(y)$. For every probability distribution you can think of we can define the entropy

$$S = \int p(x|y) \ln(p(x|y)) \tag{9.15}$$

that is the relative information of x with respect to y (dimensionless / natural units / units of bits). So $\frac{S}{\ln(2)}$ is the average number of yes / no questions to infer x if only y is known.

In information theory you define a piece of information as 1 nat $= \ln(2)^{-1}$ bits. Rescaling by $\ln(2)$ is equivalent to defining the entropy instead using the binary logarithm.

Properties of Non-Equilibrium Systems

- non-generic steady states possible (e.g. circular currents)
- small number of non-equilibrium fluctuation theorems is available

Derivation of the Boltzmann distribution

Lets consider a system with $\langle E \rangle = U$ for the canonical ensemble, which is contact with some heath bath of temperature T. As a trick we map the it to a microcanonical ensemble of N independent systems with N_i system in an energy state E_i.

Now we have two constraints:

i) $\sum_i N_i = N$

ii) $\sum_i N_i E_i = NU$

Then we introduce the weight function W from statistical physics and count how many compatible microstates there are for a given set $\{N_i\}$. Doing simple combinatorics we get

$$W = \frac{N!}{N_1!N_2!\dots} \tag{9.16}$$

The macrostate with maximum W is most probable, but we need to take into account the constraints. So the way to go is to introduce Lagrange multipliers. We know that

$$0 = \mathrm{d}\ln(W) = \sum_i \frac{\partial \ln(W)}{\partial N_i}\,\mathrm{d}N_i + \alpha \sum \mathrm{d}N_i - \beta \sum E_i\,\mathrm{d}N_i \tag{9.17}$$

so

$$\frac{\partial \ln(W)}{\partial N_i} + \alpha - \beta E_i = 0 \tag{9.18}$$

with

$$\frac{\partial \ln(W)}{\partial N_i} \overset{\text{Stirling}}{=} \frac{\partial N_j \ln(N_j)}{\partial N_i} - \sum_j \frac{\partial N \ln(N)}{\partial N_i} = \dots = -\ln\left(\frac{N_i}{N}\right) \tag{9.19}$$

so $p_i = \frac{N_i}{N} = \exp(\alpha - \beta E_i)$. You can play this game also for the grand canonical ensemble with a third condition for the mean particle number.

9.4 Thermal Fluctuations: Space-dependent Diffusion

Our diffusion coefficient now depends on the position $D = D(x)$ and we write down a Langevin equation

$$\gamma\dot{x} = -\frac{\partial U}{\partial x} + \gamma\xi(t) \tag{9.20}$$

and we have Gaussian white noise with a position-dependent noise strength $\langle \xi(t)\xi(t')\rangle = 2D(x)\delta(t-t')$. So far we can't tell whether to use Stratonovich or Ito calculus.

Starting with the Einstein relation $D = \frac{k_B T}{\gamma}$ we can distinguish two cases:

i) $\gamma = \gamma(x)$ and $T = T_0$ (equilibrium system, just passive obstacles by γ!)

ii) $\gamma = \gamma_0$ and $T = T(x)$ (non-equilibrium system!)

α-calculus

$(\alpha)\,\dot{x} = f(x) + \alpha g(x)$ with $\alpha = 0$ for Ito and $\alpha = \frac{1}{2}$ for Stratonovich. This determines what the Fokker-Planck equation looks like

$$\dot{P} = \frac{\partial}{\partial x}\left[-(f + \frac{\alpha}{2}\frac{\partial^2 g}{\partial 2^2})P + \frac{1}{2}\frac{\partial}{\partial x}\left(g^2 P\right)\right] \tag{9.21}$$

Case i): Equilibrium System

For case i) it can be shown that $\alpha = 1$ is correct (isothermal interpretation) (see Lau & Lubensky paper PRE).

$$\dot{P} = \frac{\partial}{\partial x}\left[-(f + \frac{\partial^2 g}{\partial 2^2})P + \frac{1}{2}\frac{\partial}{\partial x}\left(g^2 P\right)\right] \tag{9.22}$$

with $f = -\frac{1}{\gamma}\frac{\partial U}{\partial x}$, $g = \sqrt{2D}$ so

$$\dot{P} = -\vec{\nabla}(fP) + \vec{\nabla}(D(x)\vec{\nabla}P) \tag{9.23}$$

so this is the correct generalization of Fick's law for equilibrium systems with $\gamma = \gamma(x)$. So at the steady state we must have $\dot{P}^* = 0$ and $fP) + D(x)\vec{\nabla}P = \text{const}$ and we get the Boltzmann distribution $P^* \sim \exp(-\beta U)$.

Nota Bene

In Ito interpretation with $\alpha = 0$ we would have obtained the Fokker-Planck equation

$$\dot{P} = -\vec{\nabla}(fP) + \vec{\nabla}^2(DP) \tag{9.24}$$

which gives rise to different physics and different steady state distributions. So it is really important where to write D!

Case ii): Position-dependent Temperature

These systems behave non-generically and are characterized by thermophoreses (Sorret effect) and the Fokker-Planck equation

$$\dot{P} = -\vec{\nabla}(f - D_T\vec{\nabla}T)P + \vec{\nabla}(D(x)\vec{\nabla}P) \tag{9.25}$$

with the Sorret coefficient $S_T = \frac{D_T}{D}$, which depends on molecular interaction potentials. The Sorret effect is an example of an non-equilibrium phenomenon.

9.5 Entropy Production

A hallmark of non-equilibrium systems is entropy production, which we know from the second law of thermodynamics $\langle \Delta S \rangle \geq 0$.

As an example lets consider to systems of temperature T_1 and T_2 that are brought into contact resulting in an entropy change

$$\frac{\Delta S}{k_B} = \Delta Q(\frac{1}{k_B T_2} - \frac{1}{k_B T_1}) \tag{9.26}$$

Or consider a second example of two ideal gases with N_A and N_B particles that are mixing: $N = N_A + N_B$, $x = \frac{N_A}{N}$ and

$$\frac{\Delta S}{k_B} = -N[x\ln(x) + (1-x)\ln(1-x)] \tag{9.27}$$

as the mixing entropy.

Fluctuation Theorem of Non-Equilibrium Systems

The change of entropy will be a stochastic variable with

$$\frac{P\left(\frac{\Delta S}{k_B} = I\right)}{P\left(\frac{\Delta S}{k_B} = -I\right)} = \exp(I) \tag{9.28}$$

for a colloidal particle driven by optical tweezers a decrease in entropy might be observed, for larger system it gets really unlikely due to the exponential factor $\exp(I)$.

Crooke Fluctuation Theorem

Lets consider a macroscopic observable y so we can ask how likely it is to observe the time-reversed macroscopic dynamics / trajectory

$$\frac{P(y)}{P(\bar{y})} = \exp(\Delta S[y(t)]/k_B) \tag{9.29}$$

Jarzynski Relation

For an isolated system there is always an adiabatic process connecting y_0 and y_1 costing the work $W = \Delta F$ as change in the free energy. Any non-adiabatic process will take more work $\langle \Delta F \rangle \leq W$ and we have

$$\exp(-\Delta F) = \langle \exp(-\beta W) \rangle \tag{9.30}$$

10 Decision Theory

Consider a (biomedical) variable z which will have different statistics $P(z|s_1)$ and $P(z|s_2)$, respectively, for the two states s_1 meaning "healthy" and s_2 meaning "'ill"'.

So our task is now to decide between the options d_1(guess s_1) and d_2(guess s_2). So we can have a look at the likelihood ration

$$\Lambda = \frac{P(z|s_1)}{P(z|s_2)} \tag{10.1}$$

and employ a maximum-likelihood test

to decide for d_1 if $P(z|s_1) > P(z|s_2)$, i.e. $\Lambda > 1$ to decide for d_2 if $P(z|s_2) > P(z|s_1)$, i.e. $\Lambda < 1$

There are different types of errors

$P(d_2|s_1)$ = Type-I error (false alarm / false positive error)

$P(d_1|s_2)$ = Type-II error (false negative error / a building is burning, but the fire alarm is not set off)

Any statistical test can be characterized by its Receiver of Operating Characteristics (ROC)

Bayes Risk Criterium

We have a cost matrix with $\hat{c} = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}$ and c_{ij} cost of d_i if s_j true c_{12} cost of d_1 if s_2 true

and the base rates $P(s_1)$, $P(s_2) = 1 - P(s_1)$

so now we can calculate an expected cost

$$\langle c \rangle = c_{11}P(d_1|s_1)P(s_1) + c_{12}P(d_1|s_2)P(s_2) + \dots \tag{10.2}$$

so an optimal test for the likelihood ratio would be

$$\Lambda(z) = \frac{P(z|s_2)}{P(z|s_1)} \overset{d_1 d_2}{<>} \frac{(c_{21} - c_{11})P(s_1)}{(c_{12} - c_{22})P(s_2)} = \theta \tag{10.3}$$

Example: $c_{12} \to \infty$ then $\theta \to 0$ and always d_2 is chosen

Lets calculate an expected cost for the optimal test, so depending on the base probability $P_0 = P(s_2)$ what is the cost $c(P_0)$? –> GRAPHICS

Generalizations

- vector observations with z_1, z_2
- multiple decisions

Sequential Bayes Test

We can either decide for d_1, d_2 or ? which means undecided.

When zero measurements are made we have

$$\Lambda_0 = \frac{P(s_2)}{P(s_1)} \tag{10.4}$$

Without loss of generality we can write $\hat{c} = \begin{pmatrix} 0 & c_{12} \\ c_{21} & 0 \end{pmatrix}$ (only the differences are relevant)

Question: So would it be beneficial to take one more measurement?

with Q_1, Q_2 are the critical base rates so that $c_{12}Q_1 = c(Q_1)+\beta$ and $c_{21}(1-Q_2) = c(Q_2)+\beta$

(Left side: cost for no measurement, right side: cost for one measurement)

$T_1 = \frac{Q_1}{1-Q_1}$ and $T_2 = \frac{Q_2}{1-Q_2}$ (corresponding likelihood ratios)

If $\Lambda_0 < T_1$ then we go for d_1, if $\Lambda_0 > T_2$ then d_2 and if in between then we take another test.

Next step: one measurement, so we can calculate an updated likelihood ratio

$$\Lambda_1(z_1) = \frac{P_1}{1-P_1} = \frac{P(s_2|z_1)}{P(s_1|z_1)} = \frac{P(z_1|s_2)P(s_2)}{P(z_1|s_1)P(s_1)} = \frac{P(z_1|s_2)}{P(z_1|s_1)}\Lambda_0 \tag{10.5}$$

so if $\Lambda_1 < T_1$ then d_1, if $\Lambda_1 > T_2$ then d_2 and if $T_1 \geq \Lambda_1 \geq T_2$ we perform the second measurement with

$$\Lambda_2(z_2) = \frac{z_2|s_2}{z_2|s_1}\Lambda_1 \tag{10.6}$$

So the assumptions are, that measurements are independent and identically distributed. So from the sequential test we get z_1, z_2, z_3 ...

10.1 Statistical Testing

Decision theory meant, that we have a number of different measurement models and we decide which one is more likely.

For statistical testing usually we have a working hypothesis H_1 and this can be formulated just qualitatively. Like H_1 = "Smoking promotes cancer.", but we don't have a measurement model.

But we can look at the Null hypothesis, i.e. the negation of our working hypothesis, $H_0 = \neg H_1$ for which we have a measurement modell $P(z)$ with measurement z if H_0 true.

For the statistical test we have a decision problem, where in the first step we accept the Null hypothesis as d_1 and reject it as d_2. And we would like to formulate a decision rule, so that for a measurement z_0 we have $P(z \geq z_0) \overset{d_2 d_1}{<>} \alpha$ with the significance level α.

Look elsewhere fallacy: if we were testing n null hypothesis $H_0^{(1)}$, $H_0^{(2)}$, ..., $H_0^{(n)}$ with fixed α then even if $H_0^{(j)}$ are true for all j an average of αn null hypothesis will be rejected.

one-sided / two-sided tests:

$\int_\theta^\infty P(z)\,\mathrm{d}z \overset{d_2 d_1}{<>} \alpha$ one-sided

$\int_{|z|\geq\theta} P(z)\,\mathrm{d}z \overset{d_2 d_1}{<>} \alpha$ two-sided

So when to go for a one-sided or two-sided test? Here the working hypothesis H_1 comes in

Example fair coin: H_0 with $p_{\text{head}} = p_{\text{tail}} = 1/2$

measurement: k-times tail after tossing n-times, so we have a measurement model

So the probability is $p(k) = 2^{-n}\binom{n}{k}$

For a one-sided test (H_0: We have a biased coin towards tail) we have

$\sum_{k=k_1}^{n} p(k) \overset{d_2 d_1}{<>} \alpha$

and for a two-sided test (H_0: we have unknown bias) we have

$\sum_{k=k_1}^{n} p(k) + \sum_{k=1}^{n-k_1} p(k) \overset{d_2 d_1}{<>} \alpha$

10.2 Student's t-test

H_0: $\langle x \rangle = \mu$ with measurement model $z = x \sim N(\mu, \sigma^2)$ with σ^2 unknown

A measurement now consists of z_1, ..., z_n and

$$t = \frac{\bar{z} - \mu}{\hat{\sigma}/\sqrt{n}} \tag{10.7}$$

so the empirical mean $\bar{z} = \frac{1}{n}(z_1 + \cdots + z_n)$ and $\hat{\sigma}^2 = \frac{1}{n-1}\sum_i (z_j - \bar{z})^2$

Nota Bene: $\bar{z} \sim N(\mu, \frac{\sigma^2}{n})$ and $\frac{\bar{z}-\mu}{\sigma/\sqrt{n}} \sim N(0,1)$

so the statistic of t is independent of μ, σ^2

The first strategy would be to perform stochastic simulations

The strategy number 2 would be to derive an analytical formula, so one can show $\bar{z} - \mu \sim N(0, \frac{\sigma^2}{n})$ and $\hat{\sigma}^2 \sim \sigma^2 \frac{\chi^2(n-1)}{n-1}$

def. χ^2-distribution: y_1, ..., $y_n \in N(0,1)$ so

$$Q = \sum_{j=1}^{n-1} y_j^2 \sim \chi^2(n-1) \tag{10.8}$$

Note: $\bar{z}$ and $\hat{\sigma}^2$ are independent

def. t-distribution

The case that $t = \frac{A}{B}$ with $A \sim N(0,1)$ and $B \sim \chi^2(n-1)$

so Student went through all the algebra

10.3 Fischer's Exact: Testing categorial data for correlations

Lets consider the two categorial properties

(A) e.g. person has been skmoking

(B) e.g. person has cancer

So the doctor compiles a continguency table of absolute frequencies

	A	$\bar{A}$	
B	N_{AB}	$N_{\bar{A}B}$	N_B
$\bar{B}$	$N_{A\bar{B}}$	$N_{\bar{A}\bar{B}}$	$N_{\bar{B}}$

So our Null hypothesis H_0 reads: $p(B|A) = p(B)$

simplification: N_A, N_B and N are fixed, so there is a single degree of freedom N_{AB}

measurement model: pick N_A objects at random and then count objects with A in selection

hypergeometric distribution

$$p(N_{AB}) = \frac{\binom{N_B}{N_{AB}}\binom{N_B}{N_A - N_{AB}}}{\binom{N}{N_A}} \tag{10.9}$$

N.B.: with replacement: Binomial Distribution without relacement: Hypergeometric Distribution

one-sided test: (suppose $k > \frac{N_A}{N} N_B$)

$$\sum_{n=N_{AB}}^{N_A} p(k) < \alpha \tag{10.10}$$

10.4 Estimation Theory

We have a measurement model with $p(z|x)$ with the measurement z and some unknown parameter x.

Maximum-likelihood estimate: $\hat{x} = argmax p(z|x)$

later: Bayesian prior $p(x)$

Warm-Up Example

How to combine noisy measurements? Suppose we have two methods 1 and 2 to measure x.

we have $p(z_1|x) \sim N(x, \sigma_1^2)$ and $p(z_2|x) \sim N(x, \sigma_2^2)$

Maximum-likelihood estimate for x:

$p(z_1, z_2|x) = p(z_1|x)p(z_2|x) \to max$

we take a product of two Gaussians and get the weighted mean

$$\hat{x} = \frac{\sigma_2^2}{\sigma_1^2 + \sigma_2^2} z_1 + \frac{\sigma_1^2}{\sigma_1^2 + \sigma_2^2} z_2 \tag{10.11}$$

Bayes formula

$$P(x|z) = \frac{P(z|x)P(x)}{P(z)} \tag{10.12}$$

$P(x)$: prior knowledge, $P(z) = \int P(z|x)P(x)\,\mathrm{d}x$ $P(z|x)$: measurement model, $P(x|z)$: a-posteriori probability distribution

Example:

$P(x) \sim N(0, \sigma^2)$, $P(z|x) \sim N(x, \theta^2)$ $P(z) \sim N(0, \sigma^2 + \theta^2)$ $P(x|z) \sim N(\hat{x}, \rho^2)$

with $\hat{x} = \frac{1}{1+\frac{\theta^2}{\sigma^2}} z = \frac{\theta^2}{\sigma^2 + theta^2} 0 + \frac{\sigma^2}{\sigma^2 + theta^2} z$

$\rho^2 = \frac{1}{\frac{1}{\sigma^2}+\frac{1}{\theta^2}}$

Curve Fitting as Estimation Problem

data points: $x_i = f(\alpha)$ with unknown parameter α

suppose we have just a set of noisy measurements $z_i = x_i + \xi_i \sim N(x_i, \sigma_i^2)$

Now we can ask for the likelihood for an observation:

$P(z_i|\alpha) \to max$ for $\alpha = \hat{\alpha}$

Assume: all measurements independent of each other

$P(\{z_i\}|\alpha) = \prod_{i=1}^{k} N_{z_i}(f_i(\alpha, \sigma^2)) \sim \exp\left[-\sum_{i=1}^{k} \frac{(f_i(\alpha)-z_i)^2}{2\sigma^2}\right]$

so $\hat{\alpha}$ minimizes th sum of square errors $\sum_{i=1}^{k}(f_i(\alpha) - z_i)^2$

so this is equivalent to a least-square fit

Generalizations:

- suppose we have different σ_i^2: weighted least-square fit, weight is $1/\sigma_i^2$

- suppose we have non-Gaussian noise in our measurement model: do maximum likelihood estimate that maximize $P(\{z_i\}|\alpha)$

10.5 Kalman Filters

We have a state space $\vec{x}_k = \vec{x}(t_k)$ e.g. position and velocity of a spaceship.

Previous estimate for $\hat{x}_{k-1}$ with covariance ellipse and then we can propagate our model forward obtaining $\hat{x}_k$

so at every time step: how to combine the previous estimate and the new measurement optimally?

Notation:

$\hat{x}_{k-1|k-1}$: previous estimate of state at time t_{k-1} $P_{k-1|k-1}$: covariance matrix of this estimate

predict step

$\hat{x}_{k|k-1}$: a-priori estimate of state at time t_k $P_{k|k-1}$: covariance matrix of this estimate

measurement step: z_k

combined into: update step htta provides a weighted average $\hat{x}_{k|k}$ a-priori estimate $P_{k|k}$: covariance matrix

Process Model: describes time evolution of our system / assume linear dynamics

$\vec{x}_k = \hat{F}_k \cdot \vec{x}_{k-1} + \vec{w}_k$

with the time-propagator $\hat{F}_k$ and the process noise $\vec{w}_k \sim N(0, \hat{Q}_k)$

Measurement Model

$\vec{z}_k = \hat{H}_k \cdot \vec{x}_k + \vec{v}_k$

measurement matrix $\hat{H}_k$ measurement noise $\vec{v}_k \sim N(0, \hat{R}_k)$

N.B. without loss of generality we can set $\hat{H} =$

Prediction Step

$\hat{x}_{k|k-1} = \hat{F}_k \cdot \vec{x}_{k-1|k-1}$ $P_{k|k-1} = \hat{F}_k P_{k-1|k-1} \hat{F}_k^T + \hat{Q}_k$

Measure $\vec{z}_k$

pre-fit residual / innovation $\vec{y}_k = \vec{z}_k - \hat{H}_k \cdot \vec{x}_{k|k-1}$

covariance pf $\vec{y}_k$: $\hat{S}_k = \hat{R}_k + \hat{H}_k P_{k|k-1} \hat{H}_k^T$

Update Step

$\hat{x}_{k|k} = \hat{x}_{k|k-1} + \hat{K}_k \vec{y}_k$ weighted average

$P_{k|k} = (\hat{I} - \hat{K}_k \hat{H}_k) P_{k|k-1} (\hat{I} - \hat{K}_k \hat{H}_k)^T + \hat{K}_k \hat{R}_k \hat{K}_k^T$

Optimal Kalman Gain

$\hat{K}_k = P_{k|k-1} \hat{H}_k^T \hat{S}_k^{-1}$

generalizes the warm-up example as ration of covariances

Theorem

The optimal Kalman gain has the following property: it minimizes the expectation value of the L^2-norm $E||\vec{x}_k - \hat{\vec{x}}_{k|k}||^2$

Proof

$E||\vec{x}_k - \hat{\vec{x}}_{k|k}||^2 = tr\hat{P}_{k|k}$

so

$0 =! \frac{\partial tr\hat{P}_{k|k}}{\partial \hat{K}_k}$

so

$\frac{\partial trAB}{\partial A} = B^T$ because $\left(\frac{\partial trAB}{\partial A}\right)_{ij} = \frac{\partial trAB}{\partial A_{ij}} = \frac{\partial tr\sum_k (AB)_{kk}}{\partial A_{ij}} = \frac{\partial tr\sum_{k,l} A_{kl}A_{lk}}{\partial A_{ij}} = B_j$

similarly: $\frac{\partial trBA^T}{\partial A} = B$

Now: $tr\hat{P}_{k|k} = tr\hat{P}_{k|k-1} - \hat{K}_k\hat{H}_k\hat{P}_{k|k-1} - \hat{P}_{k|k-1}(\hat{K}_k\hat{H}_k)^T + \hat{K}_k\hat{H}_k\hat{P}_{k|k-1}(\hat{K}_k\hat{H}_k)^T + \hat{K}_k\hat{R}_k\hat{K}_k^T$

$\frac{\partial trP_{k|k}}{\partial \hat{K}_k} = -2\hat{P}_{k|k-1}^T\hat{H}_k + 2\hat{K}_k\hat{S}_k$