STATISTICAL MECHANICS PROBLEM SETS

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Contents

Problem Set I

Exercise I.0.1.

An urn contains 4 numbered tokens from 1 to 4. After two extractions, consider the composite event $2 \cap 4$ consisting in extracting first the token 2 and then the token 4. Compute the probability $p(2 \cap 4)$:

1. If the first token is not put back into the urn after being extracted

$$D_{n,k} = \frac{n!}{(n-k)!} \longrightarrow D_{4,2} = \frac{4!}{(4-2)!} = 12$$

$$p(2 \cap 4) = \frac{1}{12} = \boxed{8.33\%}$$

2. If the first token is put back in the urn after being extracted

$$D^R_{n,k} = n^k \longrightarrow D^R_{4,2} = 4^2 = 16$$

$$p(2 \cap 4) = \frac{1}{16} = \boxed{6.25\%}$$

Exercise I.0.2

Assume that two factories A and B are the only ones in a certain market to produce trousers. A produces twice as many trousers as B. The probability for A to produce a faulty trouser is equal to $\frac{1}{5}$ and the probability for B to produce a faulty one is equal to $\frac{1}{20}$.

1. Calculate the probability of buying trouser coming from the B factory.

$P(A)$ = probability to purchase a trouser produced by A;
$P(B)$ = probability to purchase a trouser produced by B.

$$\begin{cases} P(\Omega) = P(A) + P(B) = 1 \\ P(A) = 2P(B) \end{cases}$$

$$P(B) = \frac{1}{3} = \boxed{33.3\%}$$

2. Calculate the probability of purchasing a faulty trouser.

$P(f)$ = probability to purchase a faulty trouser.

$$P(f|A) = \frac{1}{5}\,, \quad P(f|B) = \frac{1}{20}\,, \quad P(A) = 1 - P(B) = \frac{2}{3}$$

$$P(f) = P(f|A)P(A) + P(f|B)P(B) = \frac{1}{5}\frac{2}{3} + \frac{1}{20}\frac{1}{3} = \frac{3}{20} = \boxed{15\%}$$

3. Calculate the probability that a faulty trouser purchased has come from factory A.

$$P(A|f) = \frac{P(f|A)P(A)}{P(f)} = \frac{\frac{1}{5}\frac{2}{3}}{\frac{3}{20}} = \boxed{88.9\%}$$

Exercise I.0.3

Calculate the probability that among a group of 10 people there are at least 2 who celebrate their birthday on the same day (assuming no one was born in a leap year).

It is possible to compute the aforementioned probability by calculating the probability that there isn't a common birthday among the 10 people $p(Nb)$ and then computing its compliment $p(b) = 1 - p(Nb)$.
If we pick randomly a person, he/she will celebrate his/her birthday in a given day out of the 365 available. If we pick up a second person, he/she will have 364 good days left, because we do not want for him/her to celebrate his/her birthday in the same day of the first person. We can proceed like this for all the people till the 10^{th} person. The general formulation of this approach is as follow:

$$p(Nb) = \frac{365!}{(365)^n (365-n)!}$$

For $n = 10$ we get:

$$p(Nb) = \frac{365!}{(365)^{10}(365-10)!} = 88.3\%$$

$$p(b) = 1 - p(Nb) = \boxed{11.7\%}$$

Exercise I.0.4

A prick test (a test to detect allergic reactions to a substance) gives a positive outcome in allergic patients in 91% of cases, but gives a negative result in non-allergic patients in 86% of cases. The test is performed twice on a volunteer taken randomly from a country where it is known that 30% of the population is allergic to the substance. The two tests are independent of each other. What is the probability that the volunteer is allergic to the substance if one of the two tests gave a positive and the other negative?

$$P(\text{Positive}|\text{Allergic}) = P(\text{Pos}|\text{A}) = 91\% \longrightarrow P(\text{Neg}|\text{A}) = 9\%$$

$$P(\text{Negative}|\text{non-Allergic}) = P(\text{Neg}|\text{nA}) = 86\% \longrightarrow P(\text{Pos}|\text{nA}) = 14\%$$

From conditional probability,

$$P(A_i|B) = \frac{p(B|A_i)p(A_i)}{\sum_j p(B|A_j)p(A_j)}$$

$$P(\text{A}|\text{Pos}) = \frac{p(\text{Pos}|\text{A})p(\text{A})}{p(\text{Pos}|\text{A})p(\text{A}) + p(\text{Pos}|\text{nA})p(\text{nA})} = \frac{(.91)(.3)}{(.91)(.3) + (.14)(.7)} = 0.7358$$

$$\text{Set } P(\text{A}_2) = P(\text{A}|\text{Pos}) = 0.7358$$

$$P(\text{A}|\text{Neg}) = \frac{p(\text{Neg}|\text{A})p(\text{A}_2)}{p(\text{Neg}|\text{A})p(\text{A}_2) + p(\text{Neg}|\text{nA})p(\text{nA}_2)} = \frac{(0.09)(0.7358)}{(0.09)(0.7358) + (0.86)(0.264)} = 0.226$$

The probability that the patient is allergic,

$$\boxed{P(\text{A}) = P(\text{A}|\text{Neg}) = 22.6\%}$$

Exercise I.0.5

Given two independent variable X and Y taking values $k = 1, 2, ..., \infty$ with probability $p_k = 2^{-k}$ compute the probability that

$$P(X = k) = P(Y = k) = 2^{-k}$$

$$\sum_{n=n_0}^{\infty} x^n = \frac{x^{n_0}}{1-x}$$

1. $Y = X$

$$P(Y = X) = \sum_{k=1}^{\infty} P(X = k)P(Y = k) = \sum_{k=1}^{\infty} 2^{-2k} = \sum_{k=1}^{\infty} \left(\frac{1}{4}\right)^k = \frac{1}{3}$$

$$\boxed{P(Y = X) = \frac{1}{3}}$$

2. $X = 3Y$

$$P(X = 3Y) = \sum_{k=1}^{\infty} P(X = 3k)P(Y = k) = \sum_{k=1}^{\infty} 2^{-3k}2^{-k} = \sum_{k=1}^{\infty} \left(\frac{1}{16}\right)^k = \frac{1}{15}$$

$$\boxed{P(X = 3Y) = \frac{1}{15}}$$

Exercise I.0.6

Given the random variable X "score of two-dice throwing" find the probability distribution of X and $Y = (X-7)^2$. Plot the two distributions.

$$n = 6, k = 2, D_{n,k} = n^k = 36 \text{ dispositions}$$

The space event of each dice is given by Ω:

$$\Omega = \{⚀, ⚁, ⚂, ⚃, ⚄, ⚅\}$$

2^{nd}dice / 1^{st}dice	⚀	⚁	⚂	⚃	⚄	⚅
⚀	2	3	4	5	6	7
⚁	3	4	5	6	7	8
⚂	4	5	6	7	8	9
⚃	5	6	7	8	9	10
⚄	6	7	8	9	10	11
⚅	7	8	9	10	11	12

Table 1: Table of X "Score of two-dice thrown"

Looking at $Table$ 1 it is immediate to define the space event

$$\Omega_X = \{2, 3, 4, 5, 6, 7, 8, 9, 10, 11, 12\}$$

and compute the probability of each event:

$P_X(2) = P_X(12) = 2.9\%$
$P_X(3) = P_X(11) = 5.5\%$
$P_X(4) = P_X(10) = 8.3\%$
$P_X(5) = P_X(9) = 11.1\%$
$P_X(6) = P_X(8) = 13.9\%$
$P_X(7) = 16.6\%$

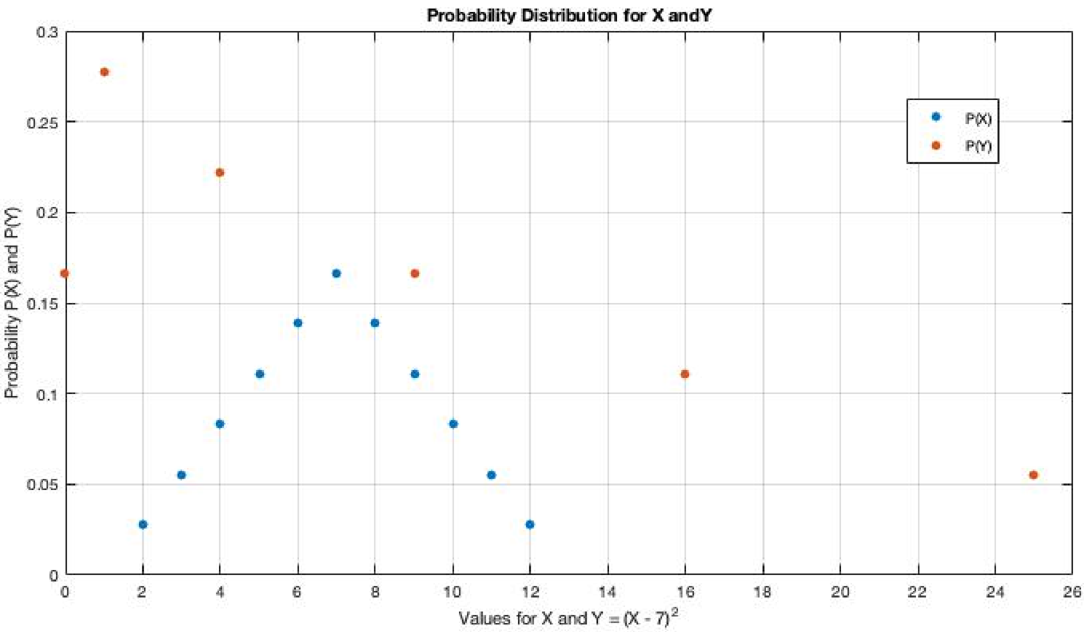
In the same way, looking at $Table$ 2 it is immediate to define the space event $\Omega_Y = \{0, 1, 4, 9, 16, 25\}$ and compute the probability of each event:

2^{nd}dice / 1^{st}dice	⚀	⚁	⚂	⚃	⚄	⚅
⚀	25	16	9	4	1	0
⚁	16	9	4	1	0	1
⚂	9	4	1	0	1	4
⚃	4	1	0	1	4	9
⚄	1	0	1	4	9	16
⚅	0	1	4	9	16	25

Table 2: Table of $Y = (X - 7)^2$

$P_Y(0) = P_Y(9) = 16.7\%$
$P_Y(1) = 27.8\%$
$P_Y(4) = 22.2\%$
$P_Y(16) = 11.1\%$
$P_Y(25) = 5.6\%$

Thus, the plot of the two distribution is as follow:



Exercise I.0.7

Rolling a dice, the success is $A = \{1, 3\}$ the failure is $\bar{A} = \{2, 4, 5, 6\}$. Calculate the probability of having 8 successes after 10 throws.

$$P_n^{(k)} = \binom{n}{k} p^k (1-p)^{n-k}$$

$$p = P(A) = \frac{2}{6} = \frac{1}{3},\ k = 8$$

$$P_{10}^{(8)} = \binom{10}{8} \left(\frac{1}{3}\right)^8 \left(1 - \frac{1}{3}\right)^{10-8} = \frac{10!}{2!\,8!} \left(\frac{1}{3}\right)^8 \left(\frac{2}{3}\right)^2 = 0.003 = \boxed{0.3\%}$$

Exercise I.0.8

Calculate the probability, after tossing a coin 4 times, to get heads at least once.

$$P(\text{at least one Heads}) = P_4^{(1)} + P_4^{(2)} + P_4^{(3)} + P_4^{(4)}$$

$$= \binom{4}{1} p^1 (1-p)^3 + \binom{4}{2} p^2 (1-p)^2 + \binom{4}{3} p^3 (1-p)^1 + p^4$$

$$= \frac{4!}{3!} \left(\frac{1}{2}\right) \left(\frac{1}{2}\right)^3 + \frac{4!}{2!\,2!} \left(\frac{1}{2}\right)^2 \left(\frac{1}{2}\right)^2 + \frac{4!}{3!} \left(\frac{1}{2}\right)^3 \left(\frac{1}{2}\right) + \left(\frac{1}{2}\right)^4 = \frac{15}{16} = \boxed{93.75\%}$$

Exercise I.0.9

The results of an experiment are described by a random variable having a uniform distribution on the support $(18.81, 18.97)$. Compute the probability, after repeating the experiment 10 times, to have 9 results within the interval $(18.84, 18.94)$.

$$f(x) = \begin{cases} \frac{1}{b-a} & a < x < b \\ 0 & \text{elsewhere} \end{cases} = \begin{cases} \frac{1}{18.97-18.81} & 18.81 < x < 18.97 \\ 0 & \text{elsewhere} \end{cases}$$

$$f(x) = \begin{cases} 6.25 & 18.81 < x < 18.97 \\ 0 & \text{elsewhere} \end{cases}$$

$$P(18.84 < x < 18.94) = \int_{18.84}^{18.94} f(x)\, dx = f(x)(18.94 - 18.84) = (6.25)(0.10) = 0.625$$

$$P_{10}^{(9)} = \binom{10}{9} (0.625)^9 (1 - 0.625) = 0.0546$$

$$\boxed{P_{10}^{(9)} = 5.46\%}$$

Exercise I.0.10

Compute the probability that in a family with 4 children:

$$P_n^{(k)} = \binom{n}{k} p^k (1-p)^{n-k}$$

$$n = 4,\ P(\text{female}) = P(\text{male}) = \frac{1}{2} = p$$

1. At least one is male

$$P(\text{at least one male}) = P_4^{(1)} + P_4^{(2)} + P_4^{(3)} + P_4^{(4)}$$

$$= \binom{4}{1} p^1(1-p)^3 + \binom{4}{2} p^2(1-p)^2 + \binom{4}{3} p^3(1-p)^1 + p^4$$

$$= \frac{4!}{3!}\left(\frac{1}{2}\right)\left(\frac{1}{2}\right)^3 + \frac{4!}{2!\,2!}\left(\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^2 + \frac{4!}{3!}\left(\frac{1}{2}\right)^3\left(\frac{1}{2}\right) + \left(\frac{1}{2}\right)^4 = \frac{15}{16} = \boxed{93.75\%}$$

2. There is at least one male and one female

$$P(\text{at least one male and one female}) = P_4^{(1)} + P_4^{(2)} + P_4^{(3)}$$

$$= \binom{4}{1} p^1(1-p)^3 + \binom{4}{2} p^2(1-p)^2 + \binom{4}{3} p^3(1-p)^1$$

$$= \frac{4!}{3!}\left(\frac{1}{2}\right)\left(\frac{1}{2}\right)^3 + \frac{4!}{2!\,2!}\left(\frac{1}{2}\right)^2\left(\frac{1}{2}\right)^2 + \frac{4!}{3!}\left(\frac{1}{2}\right)^3\left(\frac{1}{2}\right) = \frac{14}{16} = \boxed{87.5\%}$$

3. None are female.

$$P(\text{none are female}) = P(\text{all are male}) = P_4^4 = \frac{1}{16} = \boxed{6.25\%}$$

4. There is only one female

$$P(\text{only one female}) = P(\text{exactly 3 males}) = P_4^1 = P_4^3$$

$$= \frac{4!}{3!}\left(\frac{1}{2}\right)\left(\frac{1}{2}\right)^3 = \frac{1}{4} = \boxed{25\%}$$

Exercise I.0.11

X and Y are independent Poisson variables with parameter λ_1 and λ_2 respectively, i.e.

$$p(X = k) = \frac{\lambda_1^k}{k!} e^{-\lambda_1}, p(Y = k) = \frac{\lambda_2^k}{k!} e^{-\lambda_2}$$

1. Calculate $p(X + Y = k)$

If X and Y are independent Poisson variables with parameters λ_1 and λ_2 respectively, we can define a third parameter Z as a sum of X and Y with parameter λ_3 given by the sum of λ_1 and λ_2:

$$Z = X + Y \longrightarrow \lambda_3 = \lambda_1 + \lambda_2$$

$$P(X + Y = k) = P(Z = k) = \frac{\lambda_3^k}{k!} e^{-\lambda_3} = \frac{(\lambda_1 + \lambda_2)^k e^{-(\lambda_1+\lambda_2)}}{k!}$$

$$\boxed{P(X + Y = k) = \frac{(\lambda_1 + \lambda_2)^k e^{-(\lambda_1+\lambda_2)}}{k!}}$$

2. Calculate $p(X = k|X + Y = n)$:

$$P(X = k, X + Y = n) = P(X = k)P(Y = n - k)$$

$$P(X = k|X + Y = n) = \frac{P(Y = n - k)P(X = k)}{P(X + Y = n)} = \frac{\frac{\lambda_2^{n-k} e^{-\lambda_2}}{(n-k)!} \frac{\lambda_1^k e^{-\lambda_1}}{k!}}{\frac{\lambda_3^n e^{-\lambda_3}}{n!}} = \frac{n!}{k!(n-k)!} \frac{\lambda_2^{n-k} e^{-\lambda_2} \lambda_1^k e^{-\lambda_1}}{\lambda_3^n e^{-\lambda_3}}$$

$$P(X = k|X + Y = n) = \frac{\lambda_2^{n-k} \lambda_1^k e^{-(\lambda_1+\lambda_2)}}{(\lambda_1 + \lambda_2)^n e^{-(\lambda_1+\lambda_2)}} \frac{n!}{k!(n-k)!} = \left(\frac{\lambda_2}{\lambda_1 + \lambda_2}\right)^n \left(\frac{\lambda_1}{\lambda_2}\right)^k \frac{n!}{k!(n-k)!} =$$

$$\boxed{P(X = k|X + Y = n) = \frac{n!}{(n-k)!k!} \left(\frac{\lambda_1}{\lambda_1 + \lambda_2}\right)^k \left(1 - \frac{\lambda_1}{\lambda_1 + \lambda_2}\right)^{n-k}}$$

which is a binomial distribution.

Problem Set II

Exercise I.0.12

Let X be a continuous random variable with pdf

$$f(x) = \begin{cases} kx^3 & \text{for } 0 < x < 2 \\ 0 & \text{elsewhere} \end{cases}$$

1. Find the correct value of $k \in \mathbb{R}$

$$\int_{-\infty}^{\infty} dx f(x) = 1 \longrightarrow \int_0^2 dx f(x) = 1$$

$$\int_0^2 kx^3 dx = 1 \longrightarrow \frac{1}{4}k\left[x^4\right]_0^2 = 4k = 1$$

$$\boxed{k = \frac{1}{4}}$$

2. Compute $P(0.5 < x < 1)$

$$P(0.5 < x < 1) = \int_{0.5}^1 dx f(x) = \int_{0.5}^1 \frac{1}{4}x^3 dx = \frac{1}{16}(1 - 0.5^4) = 0.0586$$

$$\boxed{P(0.5 < x < 1) = 5.86\%}$$

3. Write the cumulative function

$$\boxed{F(x) = P(X \leq x) = \int_{-\infty}^{x} \frac{1}{4}x^3 dx = \begin{cases} 1, & x > 2 \\ \frac{x^4}{16}, & 0 \leq x \leq 2 \\ 0, & x < 0 \end{cases}}$$

4. Compute $\mathrm{E}[X]$ and $\mathrm{Var}[X]$

$$\mathrm{E}[X] = \int_{-\infty}^{\infty} dx f(x) x = \int_0^2 \frac{1}{4}x^4 dx = \frac{1}{20}\left[x^5\right]_0^2 = \frac{1}{20}(32) = 1.6$$

$$\boxed{\mathrm{E}[X] = 1.6}$$

$$\mathrm{Var}[X] = \int_{-\infty}^{\infty} dx f(x)(x - \mathrm{E}[X])^2 = \int_0^2 \frac{1}{4}x^3(x-1.6)^2 dx$$

$$= \frac{1}{4}\int_0^2 (x^5 - 3.2x^4 + 2.56x^3)dx = \frac{1}{4}\left[\frac{1}{6}x^6 - 0.64x^5 + 0.64x^4\right]_0^2$$

$$= \frac{1}{4}[10.667 - 20.48 + 10.24] = 0.1067$$

$$\boxed{\mathrm{Var}[X] = 0.1067}$$

Exercise I.0.13

The pdf $f_X(x)$ of the variable X is zero except in the interval $(0,1)$, where it is constant.
Compute the pdf $f_Y(y)$ of $Y = 4X(1-X)$.

$$f_X(x) = \begin{cases} h & 0 < x < 1 \\ 0 & \text{elsewhere} \end{cases}$$

In this case the function is not monotone, so one has to split the interval and study the two monotone intervals corresponding to $x < 0.5$ and $x > 0.5$:

$$|y'| = \begin{cases} +y' = -8x + 4 & \text{if } y' > 0 \\ 0 & \text{if } y' = 0 \\ -y' = 8x - 4 & \text{if } y' < 0 \end{cases} \longrightarrow \begin{cases} y' > 0 \quad \forall\, x < 0.5 \\ y' = 0 \text{ for } x = 0.5 \\ y' < 0 \quad \forall\, x > 0.5 \end{cases}$$

- $x > 0.5$. Here $x = \frac{1+\sqrt{1-y}}{2}$

$$|y'| = -4 + 8x = -4 + 8\left(\frac{1+\sqrt{1-y}}{2}\right) = 4\sqrt{1-y}$$

$$f_{Y_+}(y) = \left(\frac{f_X(x)}{\left|\frac{dy}{dx}\right|}\right) = \begin{cases} \frac{h}{4\sqrt{1-y}} & 0 < y < 1 \\ 0 & \text{elsewhere} \end{cases}$$

- $x < 0.5$. Here $x = \frac{1-\sqrt{1-y}}{2}$

$$|y'| = 4 - 8x = 4 - 8\left(\frac{1-\sqrt{1-y}}{2}\right) = 4\sqrt{1-y}$$

$$f_{Y_-}(y) = \left(\frac{f_X(x)}{\left|\frac{dy}{dx}\right|}\right) = \begin{cases} \frac{h}{4\sqrt{1-y}} & 0 < y < 1 \\ 0 & \text{elsewhere} \end{cases}$$

The pdf is obtained by summing the two parts:

$$\boxed{f_Y(y) = f_{Y_+}(y) + f_{Y_-}(y) = \begin{cases} \frac{h}{2\sqrt{1-y}} & 0 < y < 1 \\ 0 & \text{elsewhere} \end{cases}}$$

Exercise I.0.14

The pdf of the variables X and Y is

$$f(x,y) = \frac{e^{-\frac{x^2+y^2-2rxy}{2(1-r^2)}}}{2\pi\sqrt{1-r^2}}$$

where $|r| < 1$, compute the marginal pdf $f_X(x)$ and the conditional pdf $f(y|x) = \frac{f(x,y)}{f_X(x)}$ at varying r.

$f(x,y) \in R^2 \ \forall \ r \in (-1;1)$

$$f_X(x) = \int_{-\infty}^{\infty} f(x,y)dy = \frac{1}{2\pi\sqrt{1-r^2}} \int_{-\infty}^{\infty} e^{-\frac{x^2-2rxy+y^2}{2(1-r^2)}} dy$$

One can write the numerator of the exponential form of the integral as follow:

$$x^2 - 2rxy + y^2 = (y-rx)^2 + (1-r^2)x^2$$

As consequence of this, the pdf of the variables X and Y and the marginal pdf $f_X(x)$ can be written respectively as follow:

$$f(x,y) = \frac{e^{-\frac{x^2}{2}} e^{-\frac{(y-rx)^2}{2(1-r^2)}}}{2\pi\sqrt{1-r^2}}$$

$$f_X(x) = \frac{e^{-\frac{x^2}{2}}}{2\pi\sqrt{1-r^2}} \int_{-\infty}^{\infty} e^{-\frac{(y-rx)^2}{2(1-r^2)}} dy$$

Consider the change of variable $t = \frac{1}{\sqrt{2(1-r^2)}}(y-rx)$, $dt = \frac{1}{\sqrt{2(1-r^2)}}dy$, the marginal pdf $f_X(x)$ becomes

$$\boxed{f_X(x) = \frac{e^{-\frac{x^2}{2}}}{\pi\sqrt{2}} \int_{-\infty}^{\infty} e^{-t^2} dt = \frac{\sqrt{\pi}e^{-\frac{x^2}{2}}}{\pi\sqrt{2}} = \frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}}$$

The conditional pdf $f(y|x) = \frac{f(x,y)}{f_X(x)}$ is

$$f(y|x) = \frac{f(x,y)}{f_X(x)} = \frac{\frac{e^{-\frac{x^2+y^2-2rxy}{2(1-r^2)}}}{2\pi\sqrt{1-r^2}}}{\frac{e^{-\frac{x^2}{2}}}{\sqrt{2\pi}}} = \sqrt{\frac{1}{2\pi(1-r^2)}} e^{\frac{x^2}{2} - \frac{x^2-2rxy+y^2}{2(1-r^2)}} = \sqrt{\frac{1}{2\pi(1-r^2)}} e^{\frac{-x^2r^2+2rxy-y^2}{2(1-r^2)}}$$

$$\boxed{f(y|x) = \sqrt{\frac{1}{2\pi(1-r^2)}} e^{-\frac{(y-rx)^2}{2(1-r^2)}}}$$

$f(y|x)$ is the pdf associated to the distribution $N(rx, 1-r^2)$.

Exercise I.0.15

Let X_1 and X_2 be independent gaussian variables with mean value μ_1 and μ_2 and variance σ_1^2 and σ_2^2, compute the pdf of $Y = aX_1 + bX_2 + c$, where a, b and c are fixed real numbers.
The pdf of variables X_1 and X_2 are respectively:

$$f_{X_1}(x) = N(\mu_1, \sigma_1^2) \qquad f_{X_2}(x) = N(\mu_2, \sigma_2^2)$$

Since X_1 and X_2 are independent, the random variable $Y = aX_1 + bX_2 + c$ follows also the normal distribution with mean value $\mu_Y = a\mu_1 + b\mu_2 + c$ and variance $\sigma_Y^2 = a^2\sigma_1^2 + b^2\sigma_2^2$.

$$\mathrm{E}[Y] = \mu_Y = \mu_1 + \mu_2 + c$$
$$\mathrm{Var}[Y] = \sigma_Y^2 = a^2\sigma_1^2 + b^2\sigma_2^2$$

$$\boxed{f_Y(x) = N(\mu_Y, \sigma_Y^2) = \sqrt{\frac{1}{2\pi\sigma_Y^2}}e^{-\frac{(x-\mu_Y)^2}{2\sigma_Y^2}}}$$

Exercise I.0.16

Using the generating functions, show that fixing $pn = \mu$ and sending n to infinity, the Binomial distribution $p_n(k)$ tends to a Poissonian distribution.

$$P_n^{(k)} = \binom{n}{k} p^k (1-p)^{n-k} \longrightarrow \frac{e^{-\mu}}{k!}\mu^k$$

$$G(s) = \sum_{k=0}^{n} \binom{n}{k} p^k (1-p)^{n-k} s^k = (p(s-1)+1)^n$$

$$pn = \mu \to (p(s-1)+1)^n = \left(\frac{\mu}{n}(s-1)+1\right)^n$$

$$\lim_{n\to\infty} \left(\frac{\mu}{n}(s-1)+1\right)^n = e^{\mu(s-1)}$$

This is equal to the generating function for the Poisson distribution,

$$G(s) = \sum_{k=0}^{\infty} s^k \frac{\mu^k}{k!} e^{-\mu} = e^{-\mu(1-s)} = e^{\mu(s-1)}$$

Solution via limits (for our own satisfaction),

$$P_n^{(k)} = \binom{n}{k} p^k (1-p)^{n-k} = \frac{n!}{(n-k)!k!}\left(\frac{\mu}{n}\right)^k \left(1-\frac{\mu}{n}\right)^{n-k} = \frac{\mu^k}{k!}\underbrace{\frac{n!}{(n-k)!}\frac{1}{n^k}}\left(1-\frac{\mu}{n}\right)^{n-k}$$

$$\frac{n!}{(n-k)!}\frac{1}{n^k} = \frac{n(n-1)(n-2)...(n-k+1)(n-k)!}{(n-k)!n^k} = \frac{n(n-1)(n-2)...(n-k+1)}{n^k}$$

$$= \frac{n}{n}\frac{n-1}{n}\frac{n-2}{n}...\frac{n-k+1}{n} = 1\left(1-\frac{1}{n}\right)\left(1-\frac{2}{n}\right)...\left(1-\frac{k+1}{n}\right)$$

$$\frac{\mu^k}{k!}\frac{n!}{(n-k)!}\frac{1}{n^k}\left(1-\frac{\mu}{n}\right)^{n-k} = \frac{\mu^k}{k!}\left(1-\frac{1}{n}\right)\left(1-\frac{2}{n}\right)...\left(1-\frac{k+1}{n}\right)\underbrace{\left(1-\frac{\mu}{n}\right)^{n-k}}_{\left(1-\frac{\mu}{n}\right)^n\left(1-\frac{\mu}{n}\right)^{-k}}$$

$$\lim_{n\to\infty}\frac{\mu^k}{k!}\left(1-\frac{1}{n}\right)\left(1-\frac{2}{n}\right)...\left(1-\frac{k+1}{n}\right)\left(1-\frac{\mu}{n}\right)^n\left(1-\frac{\mu}{n}\right)^{-k}$$

$$= \frac{\mu^k}{k!}\underbrace{\lim_{n\to\infty}\left(1-\frac{1}{n}\right)\left(1-\frac{2}{n}\right)...\left(1-\frac{k+1}{n}\right)}_{=1}\underbrace{\lim_{n\to\infty}\left(1-\frac{\mu}{n}\right)^n}_{=e^{-\mu}}\underbrace{\lim_{n\to\infty}\left(1-\frac{\mu}{n}\right)^{-k}}_{=1}$$

$$\boxed{= \frac{\mu^k}{k!}e^{-\mu}}$$

Exercise I.0.17

Given a poissonian random variable k with parameter μ, show that in the limit of large μ the distribution tends to a gaussian with mean value μ and $\sigma^2 = \mu$.

$$p(k) = \frac{\mu^k}{k!}e^{-\mu} \text{ with } \mathrm{E}[k] = \mu \text{ and } \mathrm{Var}[k] = \mu$$

and moment-generating function

$$m_k(t) = e^{\mu(e^t - 1)}$$

$$z = \frac{k-\mu}{\sqrt{\mu}} \xrightarrow[\mu\to\infty]{} \begin{matrix}\text{continuous}\\ \text{variable}\end{matrix} \qquad \Delta z = \frac{1}{\sqrt{\mu}} \xrightarrow[\mu\to\infty]{} 0$$

$$m_z(t) = e^{-\sqrt{\mu}t} m_k\left(\frac{t}{\sqrt{\mu}}\right) = e^{-\sqrt{\mu}t} e^{\mu(e^{\frac{t}{\sqrt{\mu}}} - 1)} = e^{-\sqrt{\mu}t} e^{\mu e^{\frac{t}{\sqrt{\mu}}}} e^{-\mu}$$

Expansion of $\mu \to \infty$

$$e^{\frac{t}{\sqrt{\mu}}} \approx 1 + \frac{t}{\sqrt{\mu}} + \frac{t^2}{2\mu} + ...$$

neglecting subsequent terms for large μ

$$m_z(t) = e^{-\sqrt{\mu}t} e^{\mu e^{\frac{t}{\sqrt{\mu}}}} e^{-\mu} = \exp\left\{-\sqrt{\mu}t + \mu\left(1 + \frac{t}{\sqrt{\mu}} + \frac{t^2}{2\mu}\right) - \mu\right\}$$

$$= \exp\left\{-\cancel{\sqrt{\mu}t} + \cancel{\mu} + \cancel{\sqrt{\mu}t} + \frac{t^2}{2} - \cancel{\mu}\right\} = e^{\frac{t^2}{2}}$$

This is the moment-generating function of standard normal distribution with

$$f(x) \to g(z) = \frac{1}{\sqrt{2\pi}} e^{-\frac{z^2}{2}}$$

$$f_k = g(z)\Delta z = \frac{1}{\sqrt{2\pi}} \frac{1}{\sqrt{\mu}} e^{-\frac{(k-\mu)^2}{2\mu}}$$

With $\sigma^2 = \mu$

$$\boxed{f_k = \frac{1}{\sigma\sqrt{2\pi}} e^{-\frac{(k-\mu)^2}{2\sigma^2}}}$$

Exercise I.0.18

Find the Cramer's function for large N of the variable $Y = \frac{1}{N}\sum_{j=1}^{N} X_j$,where $\{X_j\}$are id random variables with exponential distribution

$$f(x) = \lambda e^{-\lambda x}$$

Show that the central limit theorem is recovered for small deviations.

$$m_X(t) = \lambda \int_0^\infty e^{-\lambda x} e^{tx} dx = \lambda \frac{e^{(t-\lambda)x}}{t-\lambda}\Bigg|_0^\infty = \frac{\lambda}{\lambda - t}$$

$$c_X(t) = \ln m_X(t) = \ln \frac{\lambda}{\lambda - t}$$

$$y = \frac{d}{dt} c_X(t) = \frac{d}{dt}\left[\ln \frac{\lambda}{\lambda - t}\right] = \frac{1}{\lambda - t}, \qquad t = \lambda - y^{-1}$$

$$I(y) = yt - c_X(t) = y\lambda - \ln \frac{\lambda}{\lambda - t} - 1$$

$$\boxed{I(y) = y\lambda - 1 - \ln(\lambda y)}$$

Cramer's functon is usually used to get a good approximation of the tails of events distribution, meaning for large deviations $(y-\mu) < O(\sigma)$. In this case we want to demonstrate that Cramer's function is still valid for the approximation of the events distribution close to μ, meaning for small deviations. In order to do that, we expand the Taylor's approximation around the maximum value of the distribution, where its first derivative is zero.

$$I'(y) = \lambda - \frac{1}{y} = 0 \text{ for } y = \frac{1}{\lambda}$$

$$I''(y) = \frac{1}{y^2}$$

$$I(y) \simeq (I(y))_{y=\frac{1}{\lambda}} + (I'(y))_{y=\frac{1}{\lambda}}\left(y - \frac{1}{\lambda}\right) + (I''(y))_{y=\frac{1}{\lambda}}\left(y - \frac{1}{\lambda}\right)^2 + ...$$

$$I(y) \simeq \frac{\lambda}{\lambda} - 1 - \ln\left(\frac{\lambda}{\lambda}\right) + (\lambda - \lambda)\left(y - \frac{1}{\lambda}\right) + \frac{1}{2}\lambda^2\left(y - \frac{1}{\lambda}\right)^2$$

For $y \simeq \mu_y = \frac{1}{\lambda}$ the central limit theorem is still recovered:

$$\boxed{I(y) \simeq \frac{\lambda^2}{2}\left(y - \frac{1}{\lambda}\right)^2 = \frac{(y-\mu_y)^2}{2\sigma_x^2}}$$

Problem Set III

Exercise I.0.19

Consider a system of N non-interacting harmonic oscillators of mass m and frequency ω in one dimension, described by the Hamiltonian

$$H = \sum_{j=1}^{N} \left(\frac{p_j^2}{2m} + \frac{m\omega^2}{2} q_j^2 \right),$$

-at fixed temperature T. Compute:

1. The partition function in the canonical ensemble

$$Z = \int D\mathbf{x} e^{-\beta H} = \frac{1}{N!h^N} \int \prod_{j=1}^{N} dq_j dp_j e^{-\beta H} = \frac{1}{N!h^N} \prod_{j=1}^{N} \int dq_j dp_j e^{-\beta H}$$

$$= \frac{1}{N!h^N} \left[\int dq\, dp \exp\left\{ -\frac{1}{k_B T} \left[\frac{p^2}{2m} + \frac{m\omega^2}{2} q^2 \right] \right\} \right]^N$$

$$= \frac{1}{N!h^N} \left[\int \exp\left\{ -\frac{1}{k_B T} \frac{p^2}{2m} \right\} dp \int \exp\left\{ -\frac{1}{k_B T} \frac{m\omega^2}{2} q^2 \right\} dq \right]^N$$

From the Gaussian integral

$$I_0(\alpha) = \int_{-\infty}^{\infty} dx e^{-\alpha x^2} = \sqrt{\frac{\pi}{\alpha}}$$

we have

$$Z = \frac{1}{N!h^N} \left[\sqrt{2\pi k_B T m} \sqrt{\frac{2\pi k_B T}{m\omega^2}} \right]^N = \frac{1}{N!h^N} \left[\frac{2\pi k_B T}{\omega} \right]^N$$

$$\boxed{Z = \frac{1}{N!} \left[\frac{2\pi}{\omega h \beta} \right]^N}$$

2. The Helmholtz free energy

$$F = -\frac{1}{\beta} \ln Z$$

$$\boxed{F = -\frac{1}{\beta} \ln \frac{1}{N!} \left[\frac{2\pi}{\omega h \beta} \right]^N = -k_B T \ln \frac{1}{N!} \left[\frac{2\pi k_B T}{\omega h} \right]^N}$$

3. The internal energy and its variance

$$U = \langle H \rangle = -\frac{\partial}{\partial \beta} \ln Z = -\frac{\partial}{\partial \beta} \left[\ln \frac{1}{N!} \left[\frac{2\pi}{\omega h \beta} \right]^N \right] = \frac{N}{\beta}$$

$$\boxed{U = \frac{N}{\beta} = N k_B T}$$

$$\mathrm{Var}[H] = \langle H^2 \rangle - U^2 = \frac{\partial^2}{\partial \beta^2} \ln Z = \frac{\partial}{\partial \beta} \left[-\frac{N}{\beta} \right]$$

$$\boxed{\mathrm{Var}[H] = \frac{N}{\beta^2} = N k_B^2 T^2}$$

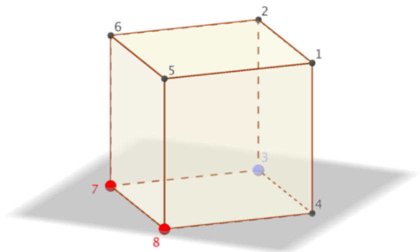
4. The entropy of the system.

$$S = -\frac{\partial F}{\partial T} = -\frac{\partial}{\partial T} \left[-k_B T \ln \frac{1}{N!} \left[\frac{2\pi k_B T}{\omega h} \right]^N \right]$$

$$\boxed{S = N k_B + k_B \ln \frac{1}{N!} \left[\frac{2\pi k_B T}{\omega h} \right]^N}$$

Exercise I.0.20

An ant is initially on the vertex 1 of the cube in the figure and it can only move from one vertex to another passing through the edge that joins them. Starting from a vertex, the ant randomly moves to one of the three neighboring first vertices with equal probability $p = \frac{1}{3}$. Some poison has been placed on the vertices 7 and 8, so if the ant arrives there it dies. Will the ant surely die? What is the probability to die at vertex 7? What is the probability to die at vertex 8?



This can be represented mathematically as a Markov chain with discrete time steps. The probability of the ant being at any vertex at the time step t_n is given by the following equation.

$$\mathbf{p}(t_n) = \mathbf{W}\mathbf{p}(t_{n-1}) = \mathbf{W}^n\mathbf{p}(t_0)$$

Where $\mathbf{W}$ is the transition matrix, and can be written explicitly as,

$$\mathbf{W} = \begin{pmatrix} 0 & \frac{1}{3} & 0 & \frac{1}{3} & \frac{1}{3} & 0 & 0 & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & 0 \\ 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 \\ \frac{1}{3} & 0 & \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} \\ \frac{1}{3} & 0 & 0 & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} \\ 0 & \frac{1}{3} & 0 & 0 & \frac{1}{3} & 0 & \frac{1}{3} & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 & 0 & 1 \end{pmatrix}$$

In order to find the probability of the ant dying at vertices 7 and 8, we must compute the probability of each state as n goes to infinity.

$$\mathbf{p}_{n\to\infty} = \lim_{n\to\infty} \mathbf{W}^n = \mathbf{T}\mathbf{W}_D^n\mathbf{T}^{-1} = \begin{pmatrix} 0 & \cdot & \cdot & \cdot & \cdot & \cdot & \frac{3}{7} & \frac{4}{7} \\ \cdot & \cdot & & & & & \frac{4}{7} & \frac{3}{7} \\ \cdot & & \cdot & & & & \frac{9}{14} & \frac{5}{14} \\ \cdot & & & \cdot & & & \frac{5}{14} & \frac{9}{14} \\ \cdot & & & & \cdot & & \frac{5}{14} & \frac{9}{14} \\ \cdot & & & & & \cdot & \frac{9}{14} & \frac{5}{14} \\ \cdot & & & & & & 1 & 0 \\ \cdot & & & & & & 0 & 1 \end{pmatrix}$$

This gives the probability of being at each state horizontally and the probability to be at those states depending on which vertex is the starting point vertically. With the ant starting at vertex 1,

$$\boxed{\begin{aligned} p(1\to 7) &= \lim_{n\to\infty} \mathbf{W}^n_{1,7} = \frac{3}{7} \\ p(1\to 8) &= \lim_{n\to\infty} \mathbf{W}^n_{1,8} = \frac{4}{7} \end{aligned}}$$

we see the the probability of dying at vertex 7 to be $\frac{3}{7}$ and the probability of dying at vertex 8 to be $\frac{4}{7}$.

Exercise I.0.21

Given a Markov chain with two states $X = \{1, 2\}$ such that

$$P_{1\to1} = 1 - p; P_{1\to2} = p; P_{2\to1} = q; P_{2\to2} = 1 - q$$

1. Find the invariant probabilities $\mathbf{p}^{st} = \binom{p_1^{st}}{1-p_1^{st}}$

   The invariant probabilities must satisfy the condition

$$\mathbf{p}_{st} = \mathbf{W}\mathbf{p}_{st} \quad \text{with} \quad \mathbf{W} = \begin{pmatrix} 1-p & q \\ p & 1-q \end{pmatrix}$$

$$\mathbf{p}^{st} = \begin{pmatrix} p_1^{st} \\ 1 - p_1^{st} \end{pmatrix} = \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

$$\mathbf{p}_{st} = \mathbf{W}\mathbf{p}_{st} \longrightarrow \begin{pmatrix} w_1 \\ w_2 \end{pmatrix} = \begin{pmatrix} 1-p & q \\ p & 1-q \end{pmatrix} \begin{pmatrix} w_1 \\ w_2 \end{pmatrix}$$

$$w_1 = (1-p)w_1 + qw_2 \qquad w_2 = pw_1 + (1-q)w_2$$

   Using $w_2 = 1 - w_1$ and $w_1 = 1 - w_2$

$$w_1 = w_1 - pw_1 + q - qw_1$$

$$q = pw_1 + qw_1 \longrightarrow w_1 = \frac{q}{p+q}$$

$$w_2 = p - pw_2 + w_2 - qw_2$$

$$pw_2 + qw_2 = p \longrightarrow w_2 = \frac{p}{p+q}$$

$$\boxed{\mathbf{p}_{st} = \frac{1}{p+q}\begin{pmatrix} q \\ p \end{pmatrix}}$$

2. Show that the detailed balance holds

   The detailed balance condition to be verified is

$$W_{ij}p_j^{st} = W_{ji}p_i^{st} \quad \forall i, j$$

   Both i and j can assume values $(1, 2)$, so that the detailed balance condition becomes:

$$W_{12}p_2^{st} = q\frac{p}{p+q}$$
$$W_{21}p_1^{st} = p\frac{q}{p+q}$$

$$W_{12}p_2^{st} = W_{21}p_1^{st}$$

<u>The detailed balance condition is verified.</u>

3. Compute the correlation function

$$\langle g(t_n)g(0)\rangle = \sum_{i,j} g_i g_j p_j P_{j\to i}(t_n)$$

   of the function g which is 1 if $i = 1$ and 0 if $i = 2$.

   Using the properties of the Markov chains

$$P_{j\to i}(t_n) = (W^n)_{ij},$$

The matrix W can be written as

$$W = TW_DT^{-1} \longrightarrow W^n = TW_D^nT^{-1},$$

with T , W_D and T^{-1} being respectively

$$T = \begin{pmatrix} \frac{q}{p} & -1 \\ 1 & 1 \end{pmatrix} \quad W_D = \begin{pmatrix} 1 & 0 \\ 0 & 1-p-q \end{pmatrix} \quad T^{-1} = \frac{p}{p+q}\begin{pmatrix} 1 & 1 \\ -1 & \frac{q}{p} \end{pmatrix}$$

We can now commute the matrix W^n:

$$W^n = TW_D^nT^{-1} = \frac{p}{p+q}\begin{pmatrix} \frac{q}{p} & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & (1-p-q)^n \end{pmatrix}\begin{pmatrix} 1 & 1 \\ -1 & \frac{q}{p} \end{pmatrix}$$

$$W^n = \begin{pmatrix} \frac{q+p(1-p-q)^n}{p+q} & \frac{q(1-(1-p-q)^n)}{p+q} \\ \frac{p(1-(1-p-q)^n)}{p+q} & \frac{p+q(1-p-q)^n}{p+q} \end{pmatrix} = \begin{pmatrix} P^{st}_{1\to1} & P^{st}_{2\to1} \\ P^{st}_{1\to2} & P^{st}_{2\to2} \end{pmatrix}$$

$$\langle g(t_n)g(0)\rangle = \sum_{i,j} g_ig_jp_j^{st}P^{st}_{j\to i} = \sum_{i,j} g_ig_j(W^n)_{ij}p_j^{st} = \sum_{i,j} g_ig_j(W^n)_{ji}p_i^{st} = \sum_{i,j} g_ig_jP^{st}_{j\to i}p_i^{st}$$

$$\langle g(t_n)g(0)\rangle = g_1g_1P^{st}_{1\to1}p_1^{st} + g_1g_2P^{st}_{1\to2}p_1^{st} + g_2g_1P^{st}_{2\to1}p_2^{st} + g_2g_2P^{st}_{2\to2}p_2^{st}$$

Remembering that $g_1 = 1$ and $g_2 = 0$, one obtains

$$\boxed{\langle g(t_n)g(0)\rangle = g_1g_1P^{st}_{1\to1}p_1^{st} = \frac{q(q+p(1-p-q)^n)}{(p+q)^2}}$$

Exercise I.0.22

Given the master equation with two states

$$\dot{p}_1 = -ap_1 + bp_2$$
$$\dot{p}_2 = \ ap_1 - bp_2$$

with $a, b > 0$

1. Given $p_1(0)$ calculate $p_1(t)$

   It is possible to write the system in a matrix form as follow:

$$\begin{pmatrix} \dot{p}_1 \\ \dot{p}_2 \end{pmatrix} = \mathbf{W}\begin{pmatrix} p_1 \\ p_2 \end{pmatrix} = \begin{pmatrix} -a & b \\ a & -b \end{pmatrix}\begin{pmatrix} p_1 \\ p_2 \end{pmatrix}$$

   This is a system of two first order homogeneous partial derivatives whose former solution is:

$$\begin{pmatrix} p_1(t) \\ p_2(t) \end{pmatrix} = e^{\mathbf{W}t}\begin{pmatrix} p_1(0) \\ p_2(0) \end{pmatrix} = e^{\mathbf{W}t}\begin{pmatrix} p_1(0) \\ 1-p_1(0) \end{pmatrix}$$

   remembering that $e^{\mathbf{W}} = e^{\mathbf{TW_DT^{-1}}}$, it is possible to compute the exponential matrix as follow

$$e^{\mathbf{W}t} = \begin{pmatrix} \frac{b}{a} & -1 \\ 1 & 1 \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & \frac{1}{e^{(a+b)t}} \end{pmatrix}\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix}\begin{pmatrix} \frac{a}{a+b} & \frac{a}{a+b} \\ \frac{-a}{a+b} & \frac{b}{a+b} \end{pmatrix} = \begin{pmatrix} \frac{a+be^{(a+b)t}}{(a+b)e^{(a+b)t}} & \frac{b(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}} \\ \frac{a(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}} & \frac{b+ae^{(a+b)t}}{(a+b)e^{(a+b)t}} \end{pmatrix}$$

$$\boxed{p_1(t) = (e^{\mathbf{W}t})_{11}p_1(0) + (e^{\mathbf{W}t})_{12}(1-p_1(0)) = \frac{b}{a+b}(1-e^{-t(a+b)}) + p_1(0)e^{-t(a+b)}}$$

2. Find the invariant probabilities $\mathbf{p}^{st} = \binom{p_1^{st}}{1-p_1^{st}}$

   The notion of invariant probabilities can be extended to the continuous time considering the stationary distribution as the limit $t \to \infty$, remembering that $p_1(0) + p_2(0) = 1$

$$\begin{pmatrix} p_1^{st} \\ p_2^{st} \end{pmatrix} = \lim_{t\to\infty}\begin{pmatrix} p_1(t) \\ p_2(t) \end{pmatrix} = \lim_{t\to\infty} e^{\mathbf{W}t}\begin{pmatrix} p_1(0) \\ p_2(0) \end{pmatrix} = \lim_{t\to\infty}\begin{pmatrix} \frac{a+be^{(a+b)t}}{(a+b)e^{(a+b)t}} & \frac{b(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}} \\ \frac{a(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}} & \frac{b+ae^{(a+b)t}}{(a+b)e^{(a+b)t}} \end{pmatrix}\begin{pmatrix} p_1(0) \\ 1-p_1(0) \end{pmatrix}$$

$$\boxed{\begin{pmatrix} p_1^{st} \\ p_2^{st} \end{pmatrix} = \frac{1}{a+b}\begin{pmatrix} b \\ a \end{pmatrix}}$$

It is easy to demonstrate the invariant probability distribution as follow:

$$e^{\mathbf{W}t}\begin{pmatrix} \frac{b}{a+b} \\ \frac{a}{a+b} \end{pmatrix} = \begin{pmatrix} \frac{a+be^{(a+b)t}}{(a+b)e^{(a+b)t}} & \frac{b(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}} \\ \frac{a(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}} & \frac{b+ae^{(a+b)t}}{(a+b)e^{(a+b)t}} \end{pmatrix}\begin{pmatrix} \frac{b}{a+b} \\ \frac{a}{a+b} \end{pmatrix} = \frac{1}{a+b}\begin{pmatrix} b \\ a \end{pmatrix}$$

3. Verify the validity of the detailed balance at any time:

$$p_1^{st}p_{1\to 2}(t) = p_2^{st}p_{2\to 1}(t).$$

$$p_1^{st}p_{1\to 2}(t) = p_1^{st}[e^{\mathbf{W}t}]_{21} = \left(\frac{b}{a+b}\right)\left(\frac{a(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}}\right) = \left(\frac{ba(e^{(a+b)t}-1)}{(a+b)^2e^{(a+b)t}}\right)$$

$$p_2^{st}p_{2\to 1}(t) = p_2^{st}[e^{\mathbf{W}t}]_{12} = \left(\frac{a}{a+b}\right)\left(\frac{b(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}}\right) = \left(\frac{ab(e^{(a+b)t}-1)}{(a+b)^2e^{(a+b)t}}\right)$$

$$\boxed{p_1^{st}p_{1\to 2}(t) = p_2^{st}p_{2\to 1}(t)}$$

4. Compute the correlation function

$$\langle f(t)f(0)\rangle = \sum_{i,j} f_i f_j p_i^{st} p_{i\to j}(t)$$

Where $f = 1$ if the system is in the state 1 and $f = -1$ if the system is in the state 2.

$$\langle f(t)f(0)\rangle = f_1f_1p_1^{st}p_{1\to 1}(t) + f_1f_2p_1^{st}p_{1\to 2}(t) + f_2f_1p_2^{st}p_{2\to 1}(t) + f_2f_2p_2^{st}p_{2\to 2}(t)$$

$$\langle f(t)f(0)\rangle = \frac{b}{a+b}\frac{a+be^{(a+b)t}}{(a+b)e^{(a+b)t}} - \frac{b}{a+b}\frac{a(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}} - \frac{a}{a+b}\frac{b(e^{(a+b)t}-1)}{(a+b)e^{(a+b)t}} + \frac{a}{a+b}\frac{b+ae^{(a+b)t}}{(a+b)e^{(a+b)t}}$$

$$\boxed{\langle f(t)f(0)\rangle = \frac{2b}{(a+b)e^{(a+b)t}}}$$

Exercise I.0.23

Consider the stationary process with stationary distribution

$$p(x) = \frac{1}{\sqrt{\pi}} e^{-x^2},$$

and conditional distribution

$$p(x_k;\tau|x_j;0) = \frac{1}{\sqrt{\pi(1-e^{-2\tau})}} e^{-\frac{(x_k - x_j e^{-\tau})^2}{(1-e^{-2\tau})}}$$

1. Show that the process satisfies the Chapmam-Kolmogorov equation

$$p(x_k;t_k|x_j;t_j) = \int_{-\infty}^{\infty} dx\; p(x_k;t_k|x;t)\; p(x;t|x_j;t_j)$$

Considering $t_j = 0$, for $\tau = t_k - t_j$ one can take an intermediate time $0 < t < t_k$ with $\tau_1 = t,\ \tau_2 = t_k - t$ so that $\tau = \tau_1 + \tau_2 = t_k$

$$\int dx\; p(x_k;t_k|x;t)\; p(x;t|x_j;t_j) = \int dx\; p(x_k;\tau_1+\tau_2|x;\tau_1)\; p(x;\tau_1|x_j;0)$$

$$= \frac{\int dx\; e^{-\frac{(x_k - x e^{-\tau_2})^2}{(1-e^{-2\tau_2})}}\; e^{-\frac{(x - x_j e^{-\tau_1})^2}{(1-e^{-2\tau_1})}}}{\sqrt{\pi^2(1-e^{-2\tau_1})(1-e^{-2\tau_2})}}$$

$$= \frac{e^{-\frac{x_k^2}{1-e^{-2\tau_2}} - \frac{x_j^2 e^{-2\tau_1}}{1-e^{-2\tau_1}}} \int_{dx} \exp\Big\{ -x^2 \frac{e^{-2\tau_2}(1-e^{-2\tau_1}) - (1-e^{-2\tau_2})}{(1-e^{-2\tau_2})(1-e^{-2\tau_1})} + x \frac{2x_k e^{-\tau_2}(1-e^{-2\tau_1}) + 2x_j e^{-\tau_1}(1-e^{-2\tau_2})}{(1-e^{-2\tau_1})(1-e^{-2\tau_2})} \Big\}}{\sqrt{\pi^2(1-e^{-2\tau_1})(1-e^{-2\tau_2})}}$$

Using the Gaussian integral formula

$$\int_{-\infty}^{\infty} e^{-ax^2+bx} = e^{\frac{b^2}{4a}} \sqrt{\frac{\pi}{a}}$$

with

$$a = \frac{e^{-2\tau_2}(1-e^{-2\tau_1}) - (1-e^{-2\tau_2})}{(1-e^{-2\tau_2})(1-e^{-2\tau_1})} \qquad b = \frac{2x_k e^{-\tau_2}(1-e^{-2\tau_1}) + 2x_j e^{-\tau_1}(1-e^{-2\tau_2})}{(1-e^{-2\tau_1})(1-e^{-2\tau_2})}$$

$$\frac{b^2}{4a} = \frac{x_k^2 e^{-2\tau_2}(1-e^{-2\tau_1})^2 + 2x_k x_j e^{-(\tau_1+\tau_2)}(1-e^{-2\tau_2})(1-e^{-2\tau_1}) + x_j^2 e^{-2\tau_1}(1-e^{-2\tau_2})^2}{(1-e^{-2\tau_1})(1-e^{-2\tau_2})(1-e^{-2(\tau_1+\tau_2)})}$$

$$\sqrt{\frac{\pi}{a}} = \sqrt{\frac{\pi(1-e^{-2\tau_1})(1-e^{-2\tau_2})}{(1-e^{-2(\tau_1+\tau_2)})}}$$

$$\frac{e^{-\frac{x_k^2}{1-e^{-2\tau_2}} - \frac{x_j^2 e^{-2\tau_1}}{1-e^{-2\tau_1}}}}{\sqrt{\pi^2(1-e^{-2\tau_1})(1-e^{-2\tau_2})}} \left(e^{\frac{b^2}{4a}} \sqrt{\frac{\pi}{a}} \right) = \frac{1}{\sqrt{\pi(1-e^{-2\tau})}} e^{-\frac{(x_k - x_j e^{-\tau})^2}{(1-e^{-2\tau})}}$$

<u>The CK condition is satisfied.</u>

2. Calculate $B(\tau) = \langle X(t+\tau)X(t) \rangle$

$$B(\tau) = \int dx\; x\, p(x_1,x_2;t,t+\tau) = \int dx\; x\, p(x_2;t+\tau|x_1;t)\, p(x_1;t)$$

$$= \frac{1}{\sqrt{\pi(1-e^{-2\tau})}} \int\int dx_1\, dx_2\, x_1\, x_2\, e^{-\frac{(x_2 - x_1 e^{-\tau})^2}{(1-e^{-2\tau})}}\; e^{-x_1^2}$$

$$= \frac{e^{-\tau}}{\sqrt{\pi}} \int dx_1\, x_1^2\, e^{-x_1^2} = \frac{1}{2} e^{-\tau}$$

$$\boxed{B(\tau) = \frac{1}{2} e^{-\tau}}$$

Exercise I.0.24

A discrete-time approximation of the Langevin equation for the Brownian motion of a grain into a viscous fluid is given by the following stochastic map

$$x_{n+1} = x_n + v_n \Delta t$$

$$v_{n+1} = \left(1 - \frac{\Delta t}{\tau_s}\right) v_n + \sqrt{\frac{2k_B T \Delta t}{m\tau_s}} w_n$$

where x_n and v_n are the position and the velocity of the grain at the time $t = n\Delta t$, the stochastic force term is given by the iid gaussian random variables $\{w_n\}$ satisfying the conditions

$$\mathrm{E}[w_n] = 0, \quad \mathrm{Var}[w_n] = \sigma_w^2 = 1$$

1. Show that the stationary value of the mean velocity is

$$\lim_{n\to\infty} \mathrm{E}[v_n] = v_{st} = 0,$$

and its variance

$$\lim_{n\to\infty} \mathrm{Var}[v_n] = \lim_{n\to\infty} \mathrm{E}[v_n^2] = \sigma_v^2 = \frac{k_B T}{m}$$

as required from the equipartition theorem.

In order to simplify calculus, let's define:

$$a = \left(1 - \frac{\Delta t}{\tau_s}\right) \qquad b = \sqrt{\frac{2k_B T \Delta t}{m\tau_s}}$$

Assuming that the initial velocity is normally distributed, meaning that its pdf is a gaussian with mean value $\mathrm{E}[v_0]$ and variance σ_0^2, we can indicate this distribution as $N(\mathrm{E}[v_0], \sigma_0)$. After one step, v_1 is still a normal distribution $N(\mathrm{E}[v_1], \sigma_1)$, since the linear combination of gaussian distributions is still a gaussian distribution. Given that, one can write

$$\mathrm{E}[v_1] = a\mathrm{E}[v_0]$$

For n steps, we get:

$$\mathrm{E}[v_n] = a^n \mathrm{E}[v_0]$$

Since $|a| < 1$, the limit behaviour for $n \to \infty$ is

$$\boxed{\lim_{n\to\infty} \mathrm{E}[v_n] = \lim_{n\to\infty} a^n \mathrm{E}[v_0] = v_{st} = 0}$$

independently on the initial distribution.

The variance behavior investigation can be conducted as follows

$$v_{n+1}^2 = a^2 v_n^2 + b^2 w_n^2 + 2ab v_n w_n$$

$$\mathrm{E}[v_{n+1}^2] = a^2 \mathrm{E}[v_n^2] + b^2 \sigma_w^2 + 2a^{n+1} b \mathrm{E}[v_0 w_n] + 2b \sum_{k=0}^{n} a^{n-k+1} \mathrm{E}[w_k] = a^2 \mathrm{E}[v_n^2] + b^2 \sigma_w^2$$

Iterating

$$\mathrm{E}[v_{n+1}^2] = a^4 \mathrm{E}[v_{n-1}^2] + (a^2 b^2 + 1)\sigma_w^2 = \dots = a^{2n+1} \mathrm{E}[v_0^2] + b^2 \sigma_w^2 \sum_{k=0}^{n} a^{2k} = a^{2n+1} \mathrm{E}[v_0^2] + b^2 \sigma_w^2 \frac{1 - a^{2(n+1)}}{1 - a^2}$$

$$\mathrm{Var}[v_n] = \mathrm{E}[v_n^2] - (\mathrm{E}[v_n])^2 = \mathrm{E}[v_n^2]$$

$$\lim_{n\to\infty} \sigma_v^2 = \lim_{n\to\infty} \mathrm{E}[v^2] = \frac{b^2\sigma_w^2}{1-a^2} = \frac{\frac{2k_BT\Delta t}{m\tau_s}}{1-\left(1-\frac{\Delta t}{\tau_s}\right)^2} = \frac{k_BT}{m}\left(\frac{2\tau_s}{2\tau_s-\Delta t}\right)$$

For large n, $\Delta t = \frac{t}{n} \to 0$, thus:

$$\boxed{\lim_{n\to\infty} \sigma_v^2 = \frac{k_BT}{m}}$$

as required from the equipartition theorem.

2. Find the stationary pdf of the velocity (**Hint**: use the characteristic functions and the fact that w_n are gaussian).

The characteristic function is

$$\phi_{n+1}(t) = \phi_n(at) + \phi_w(bt)$$

and its logarithm is

$$\ln\phi_{n+1}(t) = \ln\phi_n(at) + \ln\phi_w(bt)$$

Cumulative expansion is

$$\sum_{k=0}^{\infty}\left[\frac{C_{n+1}^{(k)}}{k!}(it)^k - \frac{C_n^{(k)}}{k!}(iat)^k - \frac{C_w^{(k)}}{k!}(ibt)^k\right] = 0$$

$$C_{n+1}^{(k)} = a^kC_n^{(k)} + b^kC_w^{(k)} = (a^k)^{n+1}C_0^{(k)} + b^kC_w^{(k)}\frac{1+a^{k(n+1)}}{1-a^k}$$

The limit of recursion is

$$C_\infty^{(k)} = \frac{b^kC_w^{(k)}}{1-a^k}$$

so the limit of the logarithm of the characteristic function is

$$\ln\phi_\infty(t) = \sum_{k=0}^{\infty}\frac{C_w^{(k)}}{(1-a^k)k!}(ibt)^k$$

If the pdf of w_n is a gaussian $g(w) = \mathcal{N}(0;1)$

$$\ln\phi_\infty(t) = -\frac{b^2}{(1-a^2)2}t^2. \quad \phi_\infty(t) = e^{-\frac{b^2t^2}{2(1-a^2)}}$$

so the invariant pdf is also gaussian with $\mu_{st} = \mathrm{E}[v] = 0$ and $\sigma_{st}^2 = \mathrm{Var}[v] = \frac{b^2}{(1-a^2)}$

The stationary pdf of the velocity is, for $n \to \infty$:

$$\boxed{f(v) = \mathcal{N}\left(0;\frac{b^2}{1-a^2}\right) = \mathcal{N}\left(0;\frac{k_BT}{m}\right) = \sqrt{\frac{m}{2\pi k_BT}}e^{-\frac{v^2m}{2k_BT}}}$$

3. Find the convergence time of v to its invariant pdf.

The coefficient a defines a characteristic time over which the velocity distribution becomes a stationary distribution. The convergence time can be computed as follows

$$\boxed{\tau_k = \frac{1}{|\ln(a)|} = \frac{1}{\left|\ln\left(1-\frac{\Delta t}{\tau_s}\right)\right|}}$$

4. For large time, in the stationary limit for the velocity (i.e. putting $\mathrm{E}[v_n] = \langle v \rangle_{st}$ and $\mathrm{Var}[v_n] = \sigma_{st}^2$), show that for $x_0 = 0$

$$\lim_{n\to\infty} \mathrm{E}[x_n] = 0,$$

$$\sigma_x^2 = \lim_{n\to\infty} \mathrm{E}[(x_n - x_0)^2] = 2\sigma_v^2 \tau_s t.$$

Consider the displacement of the particle, whose equation of motion is

$$\frac{d^2x}{dt^2} = -\gamma \frac{dx}{dt} + \sqrt{\epsilon}\eta(t)$$

with

- $\gamma = \frac{1}{\tau_s}$
- τ_s = decay time due to viscosity
- $\sqrt{\epsilon}\eta(t)$ = random force

in the overdamped limit, where the viscosity causes the acceleration to go to zero, the position is described by a Langevin equation

$$\frac{dx}{dt} = \frac{\sqrt{\epsilon}}{\gamma}\eta(t)$$

whose formal solution is

$$x(t) = x(0) + \frac{\sqrt{\epsilon}}{\gamma}\int_0^t dt' \eta(t')$$

$$\boxed{\mathrm{E}[x(t)] = x(0) = 0}$$

$$\mathrm{E}[x^2(t)] = x^2(0) + \frac{\epsilon}{\gamma^2}\int_0^t dt' \int_0^t dt'' \mathrm{E}[\eta(t')\eta(t'')] = q^2(0) + \frac{\epsilon t}{\gamma^2} = q^2(0) + \frac{2t}{m\gamma} k_B T$$

$$\boxed{\mathrm{Var}[x(t)] = \sigma_x^2 = \mathrm{E}[x^2(t)] - (\mathrm{E}[x(t)])^2 = \frac{2k_B T t}{m\gamma} = 2\sigma_v^2 \tau_s t}$$

5. Find the stationary pdf of the position and show that is equivalent to the continuous limit of the random walk with diffusion coefficient given by

$$D = \frac{\sigma_x^2}{2t} = \frac{k_B T}{m}\tau_s$$

The stationary pdf of the position can be computed considering a simplified version of the diffusion model, in which the velocity can assume only two discrete values $v_n = +v$ and $v_n = -v$. The particle will move on a discrete map of positions, $\Delta x = v\Delta t$ distanced one another. Considering the starting point as $X(0) = 0$, after a time $t = n\Delta t$ its position will be

$$X(t) = \Delta t \sum_{i=1}^{n} V_i$$

The probability $p_t(X = x)$ of finding the particle in the position $x = k\Delta X$ at time $t = n\Delta t$ will be the same probability $p_n(k)$ of doing $\frac{n+k}{2}$ jumps with $V_i = +v$ and $\frac{n-k}{2}$ jumps with $V_i = -v$ over the total n jumps, regardless of the positive and negative jumps order. Thus we have a Bernoulli distribution for the pdf pf the position given by

$$p_t(x) = \frac{1}{2^n}\binom{n}{\frac{n+k}{2}}$$

For large n and k, meaning after a large amount of steps, we can use the Stirling approximation $\log n! \simeq n\log(n) - n$ so that the position pdf becomes

$$\boxed{p_t(x) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}}$$

with diffusion coefficient

$$D = \frac{v^2 \Delta t}{2}$$

We found that the asymptotic pdf (stationary) of the position after a random walk, for a large number of steps, tends to a continuous Gaussian distribution with

$$\mathrm{E}[x_n] = 0$$

$$\mathrm{E}[x_n^2] = \sigma_x^2 = 2Dt$$

The limit of the continuous time can be derived from the M.E. governing the movement in an infinitesimal time of the particle jumping from a position to another with a constant rate λ. We can write the Markov chain as

$$(W^{dt})_{kj} \simeq \begin{cases} 1 - \lambda t & k = j \\ T_{kj} dt & k \neq j \end{cases}$$

The master equation is

$$\frac{dp_j(t)}{dt} = -\frac{\lambda}{2} \sum_k (2p_j(t) - p_{j+1}(t) - p_{j-1}(t))$$

The solution can be computed from the generating function

$$G(s,t) = \sum_{k=-\infty}^{\infty} s^k p_k(t) = e^{-\frac{\lambda}{2}(1-s-\frac{1}{s})}$$

By means of complex analysis, we can find the pdf from generating function

$$p_k(t) = e^{-\lambda t} I_{|k|}(\lambda t)$$

where $I_{|k|}$ is the modified Bessel function of order $|k|$. In the asymptotic limit of k^2 and t going to infinite and $\frac{k^2}{t}$ fixed, the pdf tends to a Gaussian

$$p_k(t) \to \frac{1}{\sqrt{2\pi\lambda t}} e^{-\frac{k^2}{2\lambda t}}$$

Given a rate $\lambda = 2D$, one obtains

$$\boxed{p_k(t) \to \frac{1}{\sqrt{4\pi Dt}} e^{-\frac{k^2}{4Dt}}}$$

which is a Gaussian distribution with

$$\mathrm{E}[x_n] = 0$$
$$\mathrm{E}[x_n^2] = \sigma_x^2 = 2Dt$$

Starting from two different approaches (Markov Chain for the discrete case and Master equation for the continuous case), we demonstrated that, for a very large number of events, we expect to find asymptotically the same result in terms of pdf.