Lecture 1

Introduction to random processes

Definition: Random Variable.
A *random variable* is a quantity which takes different values with probability $p(x)$.

Examples.
Here are some examples where the random variable is **discrete**.

- Flipping a coin: $\{0, 1\} \to p_i = 1/2$.
- Throwing dice: $\{0, 1, \ldots, 6\} \to p_i = 1/6$.
- Random number generator: $\{0, \ldots, \text{RANDMAX}\}$.

But it can also be **continuous**.

- Height, weight of students.
- Position of a certain particle.

Definition: Domain.
We define as the *domain*, the set of accessible values that a random variable can take.

Definition: PDF.
The *probability distribution function* (PDF) is a function that represents the frequency with which the variables take a specific value.

Example: Throwing a dice twice.
We consider a dice which we'll throw twice and sum the result of both cases together. Then, the domain will be $\{2, \ldots, 12\}$.

The PDF on the other hand can be described by the number of combinations in which we can obtain a certain value. Namely: $\{1, 2, 3, 4, 5, 6, 5, 4, 3, 2, 1\}$ and divide it by the total number of possible cases, which is 36.

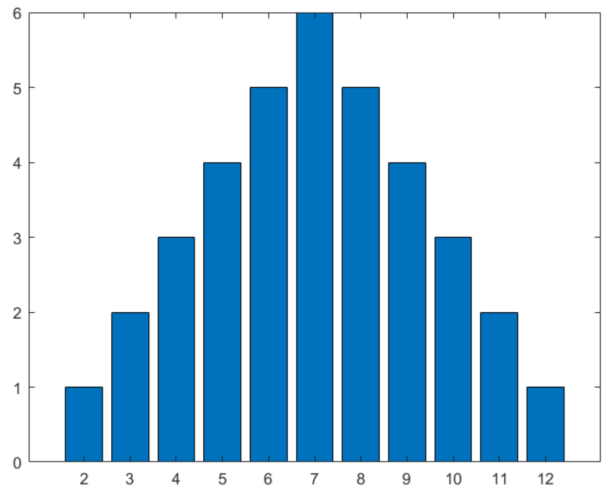

Figure 1.1: PDF of throwing 2 dice and summing the results.

Properties of p_i.
Since p_i is the probability related to a given value, we require that

1. It must be positive (or null): $p_i \geq 0$.
2. The sum of all possible probabilities is 1: $\sum_i p_i = 1$.

Definition: Continuous Random Variables.
Consider $x_i \longrightarrow x$ a continuous random variable. The probability that the variable takes a specific value is given by

$$p(x) = \lim_{\Delta x \to 0} \frac{p(\chi \in (x, x + \Delta x))}{\Delta x} \tag{1.1}$$

that is, the probability of finding a value in $(x, x + \Delta x)$ interval.

Some basic concepts and differences between discrete and continuous random variables are:

	Random Variables	
Properties	Discrete	Continuous
Domain	$\{x_1, x_2, \ldots\}$	$[a, b]$
PDF	$p_i = \text{Prob}(x = x_i)$	$p(x) = \text{Prob}(x \leq X \leq x + \Delta x)$
Cumulative function	$P_i = \text{Prob}(X < x_i)$	$P(X) = \int_a^X p(x)dx$
Positivity	$0 \leq x \leq 1$	
Bounds	[0,1]	
Normalization	$\sum_i p_i = 1$	$\int_a^b p(x)dx = 1$

Example: Uniform distribution.
Let us consider a random variable with uniform distribution and a domain between a and b. Its PDF is described as

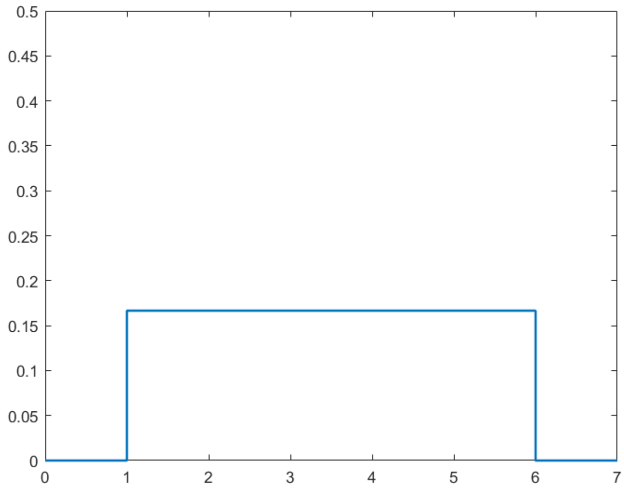

Figure 1.2: Uniform distribution graph.

The form of this function is defined as the product of two step functions:

$$p(x) = \frac{1}{b-a} \cdot \Theta(x-a) \cdot \Theta(b-x) \tag{1.2}$$

where $1/(b-a)$ is the normalization factor, and $\Theta(x)$ is defined as

$$\Theta(x) = \begin{cases} 1 & x > 0 \\ 0 & x < 0 \end{cases}$$

Then, the cumulative function results in

$$P(x) = \begin{cases} 0 & x < a \\ \frac{x-a}{b-a} & a < x < b \\ 1 & x > b \end{cases} \tag{1.3}$$

Example: Normal distribution
By definition, the normal probability distribution function is written as

$$p(x) = \frac{1}{\sqrt{2\pi}\sigma} e^{-\frac{(x-\mu)^2}{2\sigma^2}} \tag{1.4}$$

where μ, σ are the *mean* and *standard deviation* parameters, respectively. The cumulative function is defined in terms of a special function:

$$P(x) = \frac{1}{2}\left[1 + erf\left(\frac{x-\mu}{\sqrt{2}\sigma}\right)\right] \tag{1.5}$$

Definition: Moments of a PDF.
Previously we introduced the mean and standard deviation of a normal distribution without defining them properly.

The *mean value* of a probability distribution is known as the first moment of a PDF, which is calculated as:

$$\langle x \rangle = \mu = \int_a^b x \cdot p(x) dx \tag{1.6}$$

We can calculate the second moment, also known as the variance (or the square of the standard deviation), in a similar fashion:

$$\langle (x-\mu)^2 \rangle = \sigma^2 = \langle x^2 \rangle - \langle x \rangle^2 \tag{1.7}$$

In general, the n-th moment is found as

$$\langle x^n \rangle = \mu_n = \int_a^b (x-\mu)^n \cdot p(x) dx \tag{1.8}$$

Exercise:
Calculate the first and second moments of the previous examples of random distributions, and check that for the normal distribution the mean and standard deviation coincide with μ and σ respectively.

Central Value Theorem

Let us try to find the probability distribution of N mean values of $g(z)$, with

$$z = \frac{x_1 + \ldots + x_N}{N}$$

where the PDF of each x_i is $p(x)$.

$$g(z) = \int dx_1 p(x_1) \ldots \int dx_N p(x_N) \cdot \delta(z - \frac{x_1 + x_2 + \ldots + x_N}{N})$$

We can use the result that the Fourier transform of a constant is a $\delta \cdot f(x)$:

$$\frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ikx} dk = \delta(x)$$

Then, from our previous expression we see that

$$\delta(z - \frac{x_1 + \ldots + x_N}{N}) = \frac{1}{2\pi} \int_{-\infty}^{\infty} e^{ik(z-(x_1+\ldots+x_N)/N)} dk$$

and

$$g(z) = \frac{1}{2\pi} \int dk e^{ikz} \int dx_1 e^{-ikx_1/N} p(x_1) \ldots \int dx_N e^{-ikx_N/N} p(x_N)$$

We can identify the terms

$$\int dx_i e^{-ikx_i/N} p(x_i) = \langle e^{-ikx/N} \rangle$$

which are all independent and can be multiplied together as

$$\langle e^{-ikx/N} \rangle^N = \langle e^{-ikx/N + ik\mu/N} \rangle^N \cdot (e^{-ik\mu/N})^N$$

where μ is the mean of x,

$$= \langle e^{-ik(x-\mu)/N} \rangle^N e^{-ik\mu}$$

For $N \to \infty$, we can expand the previous expression in powers of $(x - \mu)$:

$$\begin{aligned}
&\approx \langle 1 - \frac{ik}{N}(x-\mu) + \frac{1}{2}\left(\frac{ik}{N}(x-\mu)\right)^2 + \ldots \rangle^N \\
&= \left(1 - \frac{ik}{N}\underbrace{(\langle x \rangle - \mu)}_{0} + \frac{1}{2}\left(\frac{ik}{N}\right)^2 \underbrace{\langle (x-\mu)^2 \rangle}_{\sigma^2} + \ldots \right)^N \\
&= (1 - \frac{1}{2}\frac{k^2\sigma^2}{N^2})^N
\end{aligned}$$

using $e^x = \lim_{N\to\infty}(1 + \frac{x}{N})^N$ we see that

$$(1 - \frac{1}{2}\frac{k^2\sigma^2}{N^2})^N \approx e^{-\frac{1}{2}\frac{k^2\sigma^2}{N}}$$

We can return now to the expression of $g(z)$ and introduce this result in order to obtain the following expression

$$g(z) = \frac{1}{2\pi}\int_{-\infty}^{\infty} dk e^{ik(z-\mu)} e^{-\frac{1}{2}\frac{k^2\sigma^2}{N}}$$

which is exactly

$$\boxed{g(z) = \frac{1}{\sqrt{2\pi N\sigma}} e^{-\frac{(z-\mu)^2}{2(\sigma/N)^2}}}$$

In other words, a normal PDF with the same mean value μ and a reduced standard deviation $\sigma/\sqrt{N}$ where N is the number of values used to calculate the average. CLT requires $N \to \infty$ for this result to be exact, but it can also be used to **provide confidence limit** of the averaged quality by calculating

$$\mu \pm \frac{\sigma}{\sqrt{N}}$$

which can also be interpreted as the statistical error. However, to reduce this error by a factor of 2, we need to increase $N \to 4N$. For this reason, reducing the variance is usually more important so as to obtain small statistical errors.

Lecture 2

Random walks

Diffusion equaiton in 1D
The diffusion equation in one dimension is defined by the formula

$$\frac{\partial p(x,t)}{\partial t} = D \cdot \frac{\partial^2 p(x,t)}{\partial t^2} \tag{2.1}$$

where D is the diffusion coefficient:

- For a quantum particle $D = \frac{\hbar^2}{2m}$.
- Here $p(x,t)$ is a PDF which quantifies the probability of a particle in $(x; x+dx)$ at time t.

Diffusion equation in 3D
The generalization in three dimensions can be done trivially by changing equation 2.1 into

$$\frac{\partial p(x,y,z;t)}{\partial t} = D\left(\frac{\partial^2 p}{\partial x^2} + \frac{\partial^2 p}{\partial y^2} + \frac{\partial^2 p}{\partial z^2}\right) \tag{2.2}$$

From now on we will identify the Laplacian as $\Delta = \partial^2/\partial x^2 + \partial^2/\partial y^2 + \partial^2/\partial z^2$.

To calculate the average value of x: $\langle x \rangle$, we will multiply and integrate eq.2.1 over all possible values as

$$\begin{aligned}\int_{-\infty}^{\infty} x\frac{\partial p}{\partial t}dx &= \int_{-\infty}^{\infty} xD\frac{\partial^2 p}{\partial x^2}dx \\ \frac{\partial}{\partial t}\int_{-\infty}^{\infty} xpdx &= \underbrace{xD\frac{\partial p}{\partial x}\bigg|_{-\infty}^{\infty}}_{0} - \underbrace{\int_{-\infty}^{\infty} D\frac{\partial p}{\partial x}dx}_{0} = 0\end{aligned}$$

which means that the time derivative of the average position is zero. Namely, $\partial\langle x\rangle/\partial t = 0$, that is to say, the $\langle x \rangle = \text{const.}$. In addition, if $\langle x(t=0)\rangle = 0$, then $\langle x(t)\rangle = 0$ for all t.

We can do the same to find the average width of the random walk $\langle x^2 \rangle$, and find

$$\frac{\partial}{\partial t}\langle x^2 \rangle = 2D$$

so, we can see that $\langle x(t)\rangle = 2Dt$, also known as Einstein's equation for the diffusion.

In 3 dimensions, we can generalize the previous expressions to

$$\langle r^2 \rangle = \langle x^2 \rangle + \langle y^2 \rangle + \langle z^2 \rangle = 6Dt \tag{2.3}$$

And analogously in 2D, $\langle r^2 \rangle = 4Dt$.

Example: Random walk in 1D
Consider a **discrete** process in which:

- The particle can move to the right and left with probability $p = 1/2$ each.
- The lattice of the problem has spacing a along the x-axis.

The master equation of this process is defined as

$$p(i, N) = \frac{1}{2}\Big[p(i+1, N-1) + p(i-1, N-1)\Big]$$

where i is the i-th lattice site and N represents the moment in time (N-th step). Notice that the position at a given step in time is given by the **sum of the neighbor positions** in the lattice in the previous moment in time.

In order to move to the continuous limit, we use the following notation: $t = N \cdot \Delta t, x = a \cdot i = \Delta x \cdot i$. We will also need to normalize the probability distribution:

$$p(x, t) = \frac{1}{a} p(i, N) \longrightarrow \sum_i p(i, N) = 1$$

So, in the continuous limit the normalization condition becomes $\int p(x, t)dx = 1$. Let us rewrite the master equation with the new notation

$$\begin{aligned} p(x,t) &= \frac{1}{2}\Big[p(x+\Delta x, t-\Delta t) + p(x-\Delta x, t-\Delta t)\Big] \\ \frac{p(x,t) - p(x, t-\Delta t)}{\Delta t} &= \frac{1}{2}\frac{\Delta x^2}{\Delta t}\left[\frac{p(x+\Delta x, t-\Delta t) + p(x-\Delta x, t-\Delta t)}{\Delta x^2}\right] \end{aligned}$$

We now take the limit $\Delta x, \Delta t \to 0$ and introduce the constant $D = \Delta x^2/2\Delta t$

$$\frac{\partial p(x,t)}{\partial t} = D\frac{\partial^2 p(x,t)}{\partial x^2} \tag{2.4}$$

From this we can see that this random walk described by the PDF satisfies the diffusion equation.

Or in other words, **the random walk can be used to solve the diffusion equation**. This is specially useful when the boundary conditions are quite complicated.

Solution of the diffusion equation in 1D and free space
Let us solve equation 2.4. For that, we will move to the conjugate space, where the position is transformed into the momentum $x \to k$, by applying the Fourier transform:

$$\mathcal{F}(p(x,t)) = \frac{1}{2\pi}\int_{-\infty}^{\infty} p(x,t)e^{ikx}dx = p(k,t)$$

One particular property of the Fourier transform is that the transform of the $m-th$ derivative is equal to

$$\mathcal{F}\left[\frac{\partial^m}{\partial x^m}p(x,t)\right] = (ik)^m p(k,t)$$

With this, if we apply Fourier transform to equation 2.4, we obtain

$$\frac{\partial p(x,t)}{\partial t} = -Dk^2 p(k,t)$$

the solution of this differential equation in momentum space is simply

$$p(k,t) = e^{-Dk^2 t}p(k,t=0) \tag{2.5}$$

To go back to coordinate space we apply the *inverse* Fourier transform to equation 2.5:

$$\begin{aligned} p(x,t) &= \mathcal{F}^{-1}[p(k,t)] \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} p(k,t)e^{-ikx}dk \\ &= \int_{-\infty}^{\infty} e^{-Dk^2t-ikx}dk \\ p(x,t) &= \frac{1}{2\sqrt{\pi Dt}}e^{-x^2 4Dt} \end{aligned} \tag{2.6}$$

that is, a Gaussian with $\sigma = \sqrt{2Dt}$. Notice that, at $t = 0$, the probability distribution resembles that of a delta function at $x = 0$, and as time goes on, the probability of finding the particle elsewhere increases.

Let us now check that the average position of the particle is the same. If we write the integral

$$\langle x \rangle = \int_{-\infty}^{\infty} x\frac{1}{2\sqrt{\pi Dt}}e^{-\frac{x^2}{4Dt}}dx = 0$$

since it is the integral of an odd function (x) times an even function (the gaussian) over a symmetric interval. If we do the same for the average width, we will see that

$$\langle x^2 \rangle = \int_{-\infty}^{\infty} x^2\frac{1}{2\sqrt{\pi Dt}}e^{-\frac{x^2}{4Dt}}dx = 2Dt$$

as expected it increases with time and is proportional to the diffusion coefficient.

Since we know that the discrete random walk is also a solution to the diffusion equation, and making use of the Central Limit Theorem; which states that summing up random variables ends up with a Gaussian probability distribution, we can infer that the sum of many random walks will result in the Gaussian distribution.

Cooking Pasta

The equation relating the temperature needed to cook pasta is also a diffusion equation:

$$\frac{\partial T(x,t)}{\partial t} = D\frac{\partial^2 T(x,t)}{\partial x^2}$$

where the temperature is a function of position and time. We know from the previous results that the average width is related with the time as $\langle x^2 \rangle \propto t$. The slope of this line corresponds to the diffusion coefficient (related to the properties of the pasta) and an offset may be added if we want the pasta to be cooked "al dente".

2.1 Exercise 2: Random walk solution of Laplace equation.

Follow these steps to implement the discrete random walk algorithm:

1. Introduce a 2D grid (10x10, 30x30, ...).
2. Begin at a point (x,y), where the value of the potential has to be estimated.
3. Take a step in a random direction along x or y.
4. Continue until an edge is reached.
5. Accumulate the value of the potential at the edge $V_{bound}(i)$. Repeat this process M times.
6. The potential will be $V(x,y) = \frac{1}{M}\sum_{i=1}^{M} V_{bound}(i)$

For the second part of the exercise we will also estimate the electric field in the grid by approximating numerically the gradient of the obtained potential $\vec{E} = -\vec{\nabla}V$, as

$$\vec{E} \approx -\left(\frac{V(x+\Delta x, y) - V(x,y)}{\Delta x} + \frac{V(x, y+\Delta y) - V(x,y)}{\Delta y}\right) = (E_x, E_y)$$

and $E = \sqrt{E_x^2 + E_y^2}$.