7 Feb

Recap:

Law of large numbers

Averaging over repeated experiments (many DoF) N

↳ true expectation values

Central limit theorem

Gaussian behaviour (probability dist.) for $N \gg 1$

↳ depends on individual means & var.

($N \approx 5$ gives good approx.)

1.5 Diffusion and the central limit theorem

1.5.1 Random walk on a line

As a more general application and illustration of the central limit theorem, let's consider the behaviour of a randomly moving object. Such **random walks** appear frequently in mathematical modelling of stochastic phenomena (including Brownian motion), and can be applied to movement through either physical space or more abstract vector spaces. They are examples of Markov processes, in which the state of the system (in this case the position of the 'walker') at any time probabilistically depends only on the system's prior state at the previous point in time—there is no 'memory' of any earlier states. The resulting sequence of system states is known as a *Markov chain*, since each state is produced from the one before, like links in a chain.

To start with a simple case, let's consider a random walker that moves only in a single spatial dimension—to the left or to the right on a line—and can only take 'steps' of a fixed length, which we can set to $\ell = 1$ without loss of generality. At each point in time, the walker takes either a step to the right (R) with probability p or a step to the left (L) with probability $q = 1 - p$. We will further assume that each step takes a constant amount of time Δt, so a walk of N steps will last for total time

$$t = N\Delta t. \tag{11}$$

As an example, for $N = 6$ a representative walk can be written as $LRLRRR$, which leaves the walker $x = 2$ steps to the right of its starting point ($x = 0$). The opposite walk $RLRLLL$ would leave the walker at $x = -2$, with negative numbers indicating positions to the left of the starting point. How many possible walks are there for $N = 6$, and what is the probability (in terms of p and q) for these particular walks $LRLRRR$ and $RLRLLL$ to occur? How many possible walks are there for general N, and what is the probability for any particular walk involving r steps to the right to occur?

$N = 6$

\# walks : 2^6 — \# : 2^N

$P(LRLRRR) = p^4 q^2$ — $P_r = p^r q^{N-r}$

$P(RLRLLL) = p^2 q^4$

We will be interested in the walker's final position x at time t after it has taken N steps. Just as for the possible gains after N spins of the roulette wheel considered in Section 1.4, there are a range of possible final positions x, each of which has some probability $P(x)$ of being realized. The key pieces of information we want to determine are the expectation value $\langle x \rangle$ and the variance $\langle x^2 \rangle - \langle x \rangle^2$ that indicates the scale of fluctuations we can expect around $\langle x \rangle$ as the N-step walk is repeated many times from the same starting point. (We reserve the variables μ and σ^2 for the mean and variance (respectively) of the single-step process, which will appear when we apply the central limit theorem in Section 1.5.3.)

Suppose the N total steps involve r steps to the right. What is the final position x of the walker in terms of N and r? Check your general answer for the cases $N = 6$ and $r = 4$, 2 considered above.

$x = (+1)r + (-1)(N-r) = 2r - N$

$(N=6,\ r=4)$: $x = 2\cdot 4 - 6 = 2$

$N=6,\ r=2$: $x = 2\cdot 2 - 6 = -2$

This relation makes it equivalent to consider either the probability P_r of taking r steps to the right, or the probability $P(x)$ of ending up at final position x. This equivalence will not hold for more general random walks in which the step length is no longer fixed and ℓ_i can vary from one step to the next.

Because the order in which steps are taken does not affect the final position x, to determine the probability $P(x)$ we have to count all possible ways of walking to x. For $N = 6$, what are all the possible walks that produce $x = 4$, and what is the corresponding probability $P(4)$? $\binom{N}{r}$

$\left.\begin{matrix} N=6 \\ x=4 \end{matrix}\right\}$ $r=5$

$\left.\begin{matrix} RRRRRL \\ RRRRLR \\ RRRLRR \\ \vdots \\ LRRRRR \end{matrix}\right\}$ $6p^5 q$

Your answer should have a factor of 6 that corresponds to the binomial coefficient $\binom{N}{r} = \binom{6}{5} = 6$. In terms of this binomial coefficient, what is the general probability P_r that an N-step walk will include r steps to the right in any order?

$P_r = \binom{N}{r} p^r q^{N-r}$

Given this probability P_r, we can apply Eqs. 2–3 to find the expectation value $\langle x \rangle$ and the variance $\langle x^2 \rangle - \langle x \rangle^2$. As a first step, what are $\langle x \rangle$ and $\langle x^2 \rangle$ in terms of the expectation values $\langle r^n \rangle = \sum_{r=0}^{N} r^n P_r$?

$$\langle x \rangle = \sum_r (2r-N) P_r = 2\langle r \rangle - N \underbrace{\sum_r P_r}_{1} = 2\langle r \rangle - N$$

$$\langle x^2 \rangle = \sum_r (2r-N)^2 P_r = 4\langle r^2 \rangle - 4N\langle r \rangle + N^2$$

Now we need to calculate the necessary $\langle r^n \rangle$. An efficient way to do so is to define the **generating function**

$$T(\theta) = \sum_{r=0}^{N} e^{r\theta} P_r. \tag{12}$$

This approach introduces a parameter θ that we subsequently remove by setting $\theta = 0$. For example, $T(0) = \sum_{r=0}^{N} P_r = 1$. What do you obtain upon taking derivatives of the generating function and then setting $\theta = 0$?

$$\frac{d}{d\theta} T(\theta) \bigg|_{\theta=0} = \sum_r \frac{d}{d\theta} e^{r\theta} P_r \bigg|_{\theta=0} = \sum_r r e^{r\theta} P_r \bigg|_{\theta=0} = \sum_r r P_r = \langle r \rangle$$

$$\frac{d^n}{d\theta^n} T(\theta) \bigg|_{\theta=0} = \sum_r r^n e^{r\theta} P_r \bigg|_{\theta=0} = \sum_r r^n P_r = \langle r^n \rangle$$

For the current case of a fixed-step-length random walk in one dimension, the probabilities P_r produce a simple closed-form expression for the generating functional:

$$T(\theta) = \sum_{r=0}^{N} e^{r\theta} P_r = \sum_{r=0}^{N} \overbrace{e^{r\theta} \binom{N}{r}}^{a} p^r q^{N-r} = \left(e^{\theta} p + q\right)^N, \tag{13}$$

making use of the binomial formula $(a+b)^N = \sum_{i=0}^{N} \binom{N}{i} a^i b^{N-i}$.

$e^{r\theta} = (e^{\theta})^r$

It's straightforward to take the necessary derivatives of Eq. 13, which simplify pleasantly since $(e^\theta p+q)\big|_{\theta=0} = p+q = 1$:

$$\frac{d}{d\theta}\left(e^\theta p+q\right)^N\bigg|_{\theta=0} = N\left(e^\theta p+q\right)^{N-1} e^\theta p\Big|_{\theta=0} = Np = \langle r\rangle$$

$$\frac{d^2}{d\theta^2}\left(e^\theta p+q\right)^N\bigg|_{\theta=0} = \left(Ne^\theta p\left(e^\theta p+q\right)^{N-1} + N(N-1)\left(e^\theta p+q\right)^{N-2} e^\theta p \cdot e^\theta p\right)\Big|_{\theta=0}$$

$$= \left(Np + pN(N-1)p\right) = Np(1+Np-p)$$

$$= Np(Np+q) = \langle r^2\rangle$$

$1-p=q$

Insert the resulting $\langle r\rangle$ and $\langle r^2\rangle$ into the relations derived above:

$$\langle x\rangle = 2\langle r\rangle - N = 2Np - N = N(2p-1)$$

$$\langle x^2\rangle - \langle x\rangle^2 = 4\langle r^2\rangle - 4\cancel{N}\langle r\rangle + \cancel{N^2} - \left(4\langle r\rangle^2 - 4\cancel{N}\langle r\rangle + \cancel{N^2}\right)$$

$$= 4\left(\langle r^2\rangle - \langle r\rangle^2\right) = 4\left(\cancel{N^2p^2} + Npq - \cancel{N^2p^2}\right)$$

$$= 4Npq$$

In the end, you should obtain

$$\langle x\rangle = N(2p-1) \qquad\qquad \langle x^2\rangle - \langle x\rangle^2 = 4Npq. \qquad (14)$$

We can check that this $\langle x\rangle$ produces the expected results in the special cases $p=0$, $1/2$ and 1, while the variance also behaves appropriately by vanishing for both $p=0$ and 1.

1.5.2 Law of diffusion

It's possible to gain a more intuitive interpretation of the results in Eq. 14 by expressing them in terms of the total time t taken by the random walk (Eq. 11). Inserting $N = t/\Delta t$ into Eq. 14,

$$\langle x\rangle = \frac{t}{\Delta t}(2p-1) = \frac{2p-1}{\Delta t}t \equiv v_{\text{dr}}t, \quad \propto t$$

we see that the *expected* final position of the walker depends linearly on time, with **drift velocity**

$$v_{\mathrm{dr}} = \frac{2p-1}{\Delta t} = \frac{N(2p-1)}{t} = \frac{\langle x \rangle}{t}. \tag{15}$$

The sign of the drift velocity indicates whether the walker is drifting to the right ($p > \frac{1}{2}$) or to the left ($p < \frac{1}{2}$). The standard deviation of the final position of the walker provides a measure of the scale of fluctuations (or 'uncertainty') around the expectation value that we should anticipate:

$$\Delta x = \sqrt{\langle x^2 \rangle - \langle x \rangle^2} = 2\sqrt{Npq} = 2\sqrt{\frac{pq}{\Delta t}}\sqrt{t}, \quad \propto Nt$$

which increases proportionally to $\sqrt{t}$. This is a particular realization of a very general result.

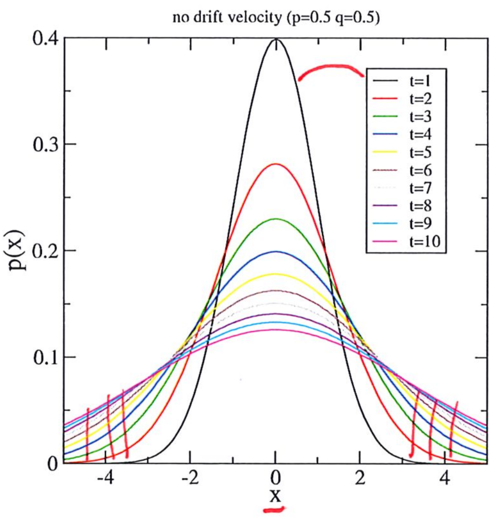
The **law of diffusion** states that

$$\Delta x = D\sqrt{t}, \tag{16}$$

where D is the **diffusion constant** and the uncertainty Δx is sometimes called the *diffusion length*.

The diffusion constant $D = 2\sqrt{\frac{pq}{\Delta t}}$ that we computed above is specific to the current case of a fixed-step-length random walk in one dimension. The behaviour it describes is illustrated by the figure below, which plots the t-dependent probability distribution $p(x)$ that we'll soon derive using the central limit theorem (Eq. 17). What we can see already, even before completing that derivation, is that the probability distribution steadily spreads out—or *diffuses*—as time passes:

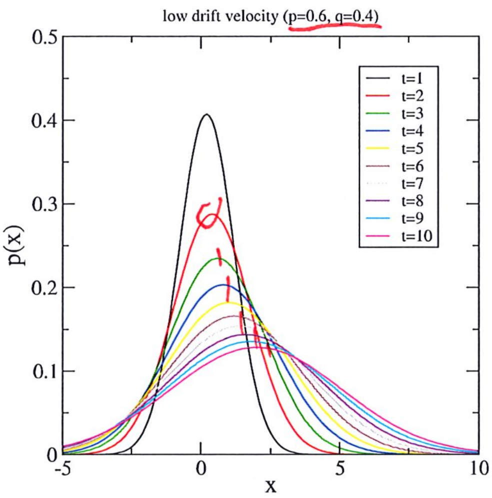
$p = q = \frac{1}{2}$

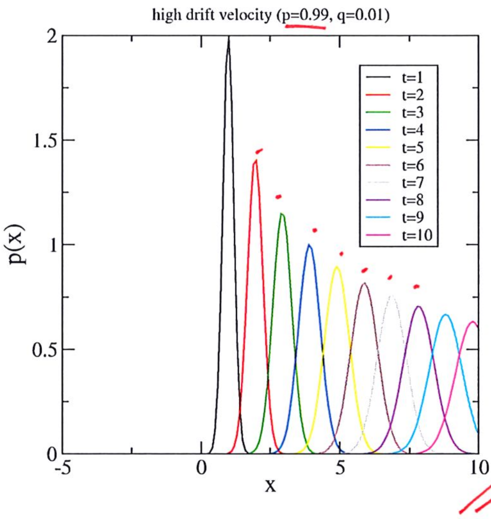


Here we are considering the special case $p = q = \frac{1}{2}$, for which the drift velocity $v_{\mathrm{dr}} = 0$ and the expectation value is always $\langle x \rangle = 0$ for any walk time t. However, as time goes on, there is a steady decrease in the probability that the walker will end up at its starting point $x = 0$. (As in Section 1.4, we can extract this probability by integrating the distribution $p(x)$ over the interval $-0.5 \le x \le 0.5$.) Instead, the interval within which we can expect to find the walker (with a constant 'one-sigma' or 68% probability) steadily grows, $-D\sqrt{t} \le x \le D\sqrt{t}$, with characteristic dependence on the square root of the time the diffusive process lasts.

Except in the trivial cases $p = 0$ or $q = 0$, diffusion also occurs when the drift velocity is non-zero. This is shown in the two figures below, considering a low but non-zero drift velocity on the left, and a high drift velocity on the right.

$V_{dr} \propto 2p-1$





7 Feb.

In the figure on the left, each individual probability distribution looks similar to the corresponding one for $v_{\text{dr}} = 0$, but now their central peaks (and expectation values $\langle x \rangle$) drift steadily to the right. The distributions in the figure on the right look a bit different, but still diffuse to exhibit shorter and broader peaks as time goes on.

When $p \neq \frac{1}{2}$ so that $\langle x \rangle \neq 0$, it is interesting to compare the drift in the expectation value against the growth in fluctuations around $\langle x \rangle$ due to diffusion. We can do this by considering the following *relative* uncertainty:

$$\frac{\Delta x}{\langle x \rangle} =$$

You should find that at large times this ratio vanishes proportionally to $1/\sqrt{t} \propto 1/\sqrt{N}$. Although the absolute uncertainty grows by diffusion, $\Delta x = D\sqrt{t}$, for $v_{\text{dr}} \neq 0$ the linear drift in the expectation value becomes increasingly dominant as time goes on.